

Documentation for PHOENICS

TR 211

The GENTRA User Guide
(Version 2006)

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*Computer Simulation of fluid flow, heat flow,
chemical reaction and stresses in solids*

The GENTRA User Guide: TR 211

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1 Introduction

1.1 What GENTRA is and does

GENTRA is a software “add-on” for the PHOENICS suite of CFD programs which provides particle-tracking facilities. The name GENTRA stands for GENeral TRacker.

GENTRA can therefore simulate the motion of particles (the “particulate or disperse phase”) through a fluid (the “continuous phase”). GENTRA takes into account the effect of the fluid velocity, temperature, turbulence, etc on the particles; and, conversely, the effect of the presence of particles on the continuous phase is also considered.

The data specification and solution procedure for the continuous phase and the particles are carried out by separate modules:

- PHOENICS is used to specify the data pertaining to the continuous phase. This can be done using any of the means available in PHOENICS (ie, PIL commands, a library case or a menu). The continuous phase thus specified is then solved by EARTH in the usual way.
- GENTRA is used to specify the data corresponding to the particulate phase. This can be done using the GENTRA menu (a part of the general PHOENICS-VR Main Menu which writes the GENTRA data at the end of the Q1 data-file), or by using in the Q1 file a subset of PIL variables specific to GENTRA. The particulate phase thus specified is then solved by GENTRA.

Of course, the solution procedures for the continuous phase and particles have to interact. Details of such interaction can be found in this manual in Section 1.4.2.

It should be pointed out that PHOENICS has already a “built-in” two-phase capability, which uses Eulerian transport equations to represent the two interacting phases (Spalding, 1980). Similarly to single-phase flows, these equations are solved by discretising the space into computational cells, by integrating the equation over each cell (thus obtaining an algebraic equation) and by solving the resulting system of algebraic equations.

The approach of GENTRA is a different one: while the continuous phase is treated as above, the particles are represented by Lagrangian equations, which are integrated to yield the particle trajectory and the particle properties along this trajectory. This approach is based on the PSI-Cell method of Crowe, Sharma and Stock (1977).

The standard two-phase PHOENICS can therefore simulate particulate flows; however, the GENTRA approach should be preferred by users who:-

- Need detailed information on the particle trajectory (eg, because particle impingement on obstacles has to be accurately predicted).
- Need to simulate accurately particle-obstacle interactions (such as bouncing, sticking or flash vaporisation).
- Have to consider simultaneously a range of particle sizes, temperatures, densities etc. (In these circumstances, the two-phase approach of PHOENICS would yield an average value for each particle property without any distribution information).
- Want to avoid numerical diffusion in the particulate phase, to which the Eulerian two-phase approach is prone, and of which the Lagrangian approach of GENTRA is free.

1.2 Features of GENTRA

The salient features of GENTRA are:-

(a) In respect of pre-processing:-

- Three alternative user interfaces for data input (menu, command language and FORTRAN);
- Full on-line help facility in the menu;
- Library of examples and test cases.

(b) In respect of modelling features:-

- GENTRA can track particles in all the co-ordinate systems supported by PHOENICS (i.e., Cartesian, cylindrical-polar and general curvilinear (BFC)).
- GENTRA can solve both steady and transient problems.
- GENTRA can model particles of six kinds:
 - (a) "Tracers" (or "lazy particles"), which simply follow the continuous-phase flow-field;
 - (b) "Beams" (or "stubborn particles"), which have a constant velocity, regardless of the continuous-phase flow field;
 - (c) Particles in isothermal flow;
 - (d) Particles experiencing heat exchange with the continuous phase;
 - (e) Melting/solidifying particles;
 - (f) Vaporising droplets.
- GENTRA will automatically detect internal walls and obstacles, and provides options for:
 - (a) Particle bouncing, with a user-specified restitution-coefficient;
 - (b) Particle adhesion to the wall;
 - (c) Withdrawal of the particle;
 - (d) Flash vaporisation of the particle (if the particle is a droplet).

(c) In respect of post-processing:

- GENTRA can generate input files for the PHOENICS post-processors VR-Viewer, PHOTON and Autoplot:
 - For VR-Viewer and PHOTON, it generates "trajectory" files, which record the trajectory of the particle as it moves through the domain.
 - For Autoplot, it generates "history files", which record the evolution of the particle properties with time.

1.3 Limitations of GENTRA

As well as capabilities, GENTRA has also limitations. Appendix A of this guide provides a list of the main limitations known to the GENTRA Development Team at CHAM. The contents of the list changes as known limitations are removed, and new ones found. An updated list of the limitations affecting **your** version of GENTRA (if different from the one described in this manual) is available through the GENTRA Input Menu (Help and information panel). See Section 2.4 of this Guide for details.

1.4 How GENTRA fits in

Section 1.1 above classified GENTRA as a PHOENICS “add-on”. The present section describes in more detail how GENTRA is related to the rest of PHOENICS.

GENTRA has a pre-processing and a processing part, which are dealt with in the following sub-sections.

1.4.1 Pre-processing

The pre-processing part involves the preparation of the GENTRA input, which consists of particle data, solution-control data and output-control data. It can be accomplished in several alternative ways:

- (a) By using the GENTRA Input Menu;
- (b) By using a set of special PIL commands (the GENTRA PIL);
- (c) By loading a case from the GENTRA Input Library.

The pre-processing side of GENTRA uses the **general** PHOENICS VR environment.

For the benefit of experienced PHOENICS users, it will be pointed out here that all the GENTRA information is sent from the Q1 file to EARTH through the “transfer” arrays RG, IG, LG, and CG.

1.4.2 Processing

The processing part of GENTRA takes the form of a collection of FORTRAN subroutines, which are attached to the PHOENICS flow-computing program, EARTH.

GENTRA, which solves the equations for the disperse phase, is called by PHOENICS between the “sweeps” of the computational domain that PHOENICS performs to solve the continuous phase. GENTRA then tracks the particles as they move through the computed flow-field, calculating in the process the interphase interactions (i.e., the transfer of momentum, mass, enthalpy, etc) between the phases. These interaction terms are, after leaving GENTRA, incorporated as sources in the continuous-phase equations for the next PHOENICS sweep.

Since the newly introduced sources are likely to alter the flow field used by GENTRA to track the particles in the first instance, several iterations of the processes PHOENICS-sweep/GENTRA-tracking will normally be needed to obtain a converged solution.

For the benefit of readers with some knowledge of the structure of EARTH, it will be pointed out here that GENTRA is attached to PHOENICS as a Ground-station subroutine that calls, in turn, all of the modules of GENTRA. Most of these modules are delivered in closed (i.e., binary) code; but the Ground station itself (called GENTRA) and a special user-accessible module (GENIUS) are provided in open source.

1.5 About this Guide

1.5.1 The purpose of this Guide, and its intended readership

This Guide has been designed to serve both as a user's guide and reference manual for GENTRA users.

GENTRA, as indeed PHOENICS, has been created to cater for the needs of users with several degrees of knowledge or experience:

- New and occasional users who want to access the system will find the GENTRA Input Menu to constitute a "fast lane"; for it can be used to set up problems with very little knowledge of PHOENICS or CFD. Chapter 2 of this document (The GENTRA Input Menu) has been provided as a guide. Its reading is, however, by no means compulsory, for most of the information it conveys is also available as on-line help to menu users.
- Expert users, or users with unusual needs, will want to know exactly what GENTRA does, and how it does it, and may wish to ascertain whether the system can be expanded, and how. For this second class of users, a "reference" element has been included in this guide, notably Chapters 3 (The GENTRA PIL), 5 (The GENTRA FORTRAN) and 6 (The GENTRA Equations).

A basic knowledge of PHOENICS and its structure is assumed in this Guide.

1.5.2 How this Guide is organised

After this introductory chapter, the reader will find the following chapters and appendices:

- Chapter 2 (The GENTRA Input Menu), which is intended mainly for beginners, describes how to use the GENTRA menu to set up particle-tracking problems.
- Chapter 3 (The GENTRA PIL) explains how more experienced users can avail themselves of a sub-set of PIL variables that circumvent the need to use the menu.
- Chapter 4 (Running GENTRA-EARTH) explains how to execute the flow-solving program, EARTH.
- Chapter 5 (The GENTRA FORTRAN) explains how experienced users can use the open-code area of GENTRA-EARTH to supplement the built-in numerical and physical features.
- Chapter 6 (The GENTRA Equations) contains a complete listing of the mathematical models embodied in GENTRA, and some details of the numerical techniques used for the solution of the equations.
- Appendix A lists the main limitations of GENTRA.
- Appendix B lists the GENTRA-PIL variables.
- Appendix C lists the user-accessible variables in the FORTRAN of GENTRA.
- Appendix D is a compilation of the GENTRA run-time errors.
- Appendix E has a listing of the Q1 file resulting from the worked example in Chapter 2.
- Appendix F has a listing of the contents of the GENTRA Input Library.
- Appendix G contains a listing of the user-accessible subroutine GENIUS.
- Appendix H is a glossary of the terms used in this manual.
- Appendix I is a list of references.
- Appendix J contains a list of the nomenclature.
- Finally, Appendix K provides information on setting up GENTRA.

1.6 Conventions used in this Guide

The following conventions are used in this Guide:-

- The **bold** typeface is used for menu titles, menu options and also for PIL variables.
- The `Courier` typeface is used for FORTRAN variables and commands.
- A pointing hand * is used in Chapter 2 to indicate comments and instructions addressed to readers who are following the worked example presented in that chapter.

2 The GENTRA Input Menu

2.1 About this chapter

As noted in Chapter 1, GENTRA is equipped with three user-interfaces:

- (a) A data-input menu;
- (b) The use of PIL commands in the Q1 file;
- (c) The use of FORTRAN in subroutine GENIUS.

This chapter explains how to use the input menu for problem specification. The use of the GENTRA Input Library of simulations is also discussed at the end of the chapter.

2.2 About the GENTRA Menu

2.2.1 What the GENTRA menu does

- (1) The GENTRA menu allows the user to specify the input data for the **disperse phase** as choices from a set of hierarchically-organised menu panels. On-line help is available to assist the user in the selection process.
- (2) The GENTRA menu makes, automatically, all the other provisions needed for the EARTH run. Chapter 3 of this Guide details the nature of these provisions for the benefit of the expert user.
- (3) The GENTRA menu writes, at the end of the current Q1 file, and as PIL commands, the results of (1) and (2) above.

2.2.2 How to access the GENTRA menu

The GENTRA menu is accessed from the '**Models**' page of the VR Main Menu, which in turn is accessed by clicking on the Menu button of the hand-set. Full details of the VR Environment are given in TR326: PHOENICS-VR Reference Guide.

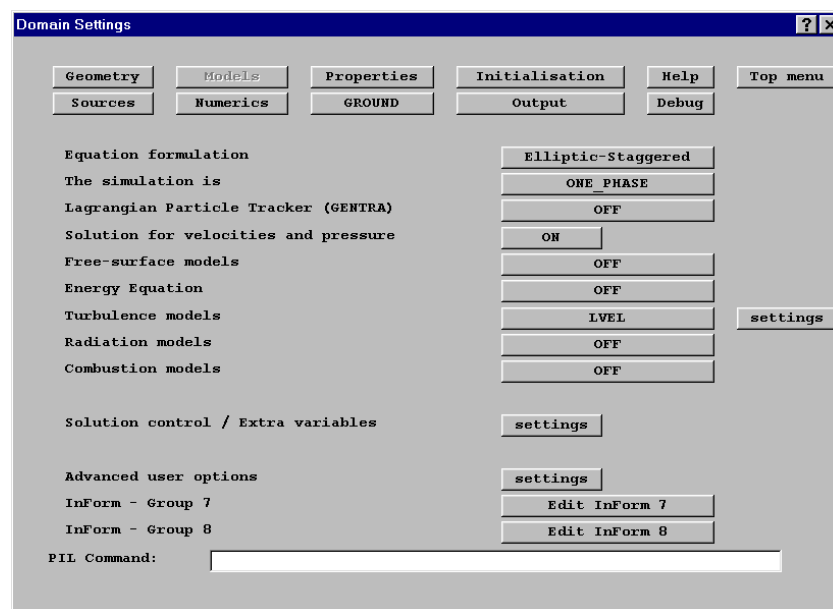


Figure 2.1 Main Menu – Models

Turn GENTRA **on** by clicking on '**OFF**' next to '**Lagrangian Particle Tracker (GENTRA)**'. A new button labelled '**Settings**' will appear. To enter the GENTRA Menu, click on '**Settings**'

2.2.3 When to call the GENTRA menu

As pointed out in Section 2.2.1, the GENTRA menu is used to specify data for the disperse phase; the user must, additionally, specify the data for the continuous phase. This can be done in any of the ways that are available in PHOENICS, for instance:

- (a) By using another menu system, such as the Main Menu;
- (b) By entering the PIL commands directly in the Q1 file; or
- (c) By loading a case from the PHOENICS Input Library.

The provisions made by the GENTRA menu will depend on the continuous-phase set-up (for instance, the auxiliary storage allocated by the GENTRA menu for the GENTRA-EARTH run will depend on the dimensionality of the problem). For this reason, you are advised to enter the GENTRA menu **after** the continuous-phase settings have been effected.

2.2.4 Obtaining help

All the menu options have associated help entries. To obtain help on an option, click the question mark "?" at the top right corner of the dialog box, then click on the item in question.

2.3 The GENTRA Main Menu panel

- * If you are following the worked example provided in this chapter, enter the PHOENICS-VR environment. Click on the **PHOENICS icon** on the desktop, or click on **Start, Programs, PHOENICS, PHOENICS**. Load the PHOENICS Library Case B534 by clicking on '**File, Load from Libraries**', entering B534 and clicking '**OK**'. This case simulates the flow of a liquid (water) through a ball valve, and will be used as the basis of the worked example. Particles (e.g., solids in suspension) will be included in the flow simulation by means of the GENTRA Input Menu.

After loading the case, you can inspect the settings by double-clicking on the various objects to bring up their Attribute dialog boxes, and check the domain settings by clicking on '**Menu**' on the hand-set.

Once you are ready to move on to GENTRA, click on '**Menu**' on the hand-set, then on '**Models**', turn GENTRA **ON** and click on '**Settings**'.

After loading the GENTRA menu as detailed in Section 2.2, the first menu panel to appear on the screen is the GENTRA Main Menu Panel, shown in figure 2.2. The options in this panel can be divided into two groups:

- The first group includes options for the entry of data of four kinds:
 - Particle physics,
 - boundary conditions for particles,
 - numerical controls and
 - input/output controls.
- The second group (with just one option) gives access to general information on GENTRA and the menu.

The options in these groups will now be explained in this manual. Section 2.4 below will explain what help and information are available on-line. Sections 2.5 to 2.9 will deal with the first group (i.e., data entry); and Section 2.10 will explain how to finish the menu session.

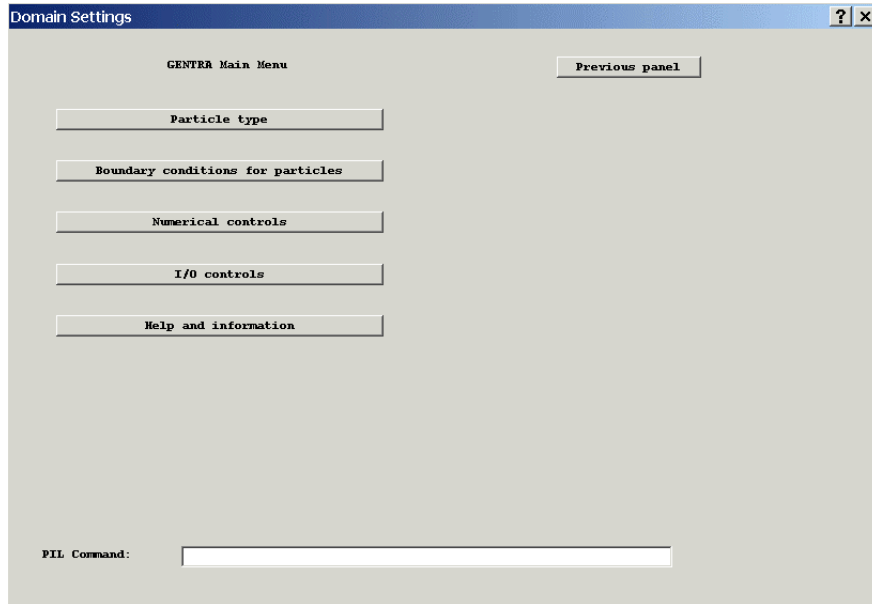


Figure 2.2: The main menu panel

2.4 Help and information

The option Help and information of the Main Menu (figure 2.2), brings up the menu panel shown in figure 2.3.

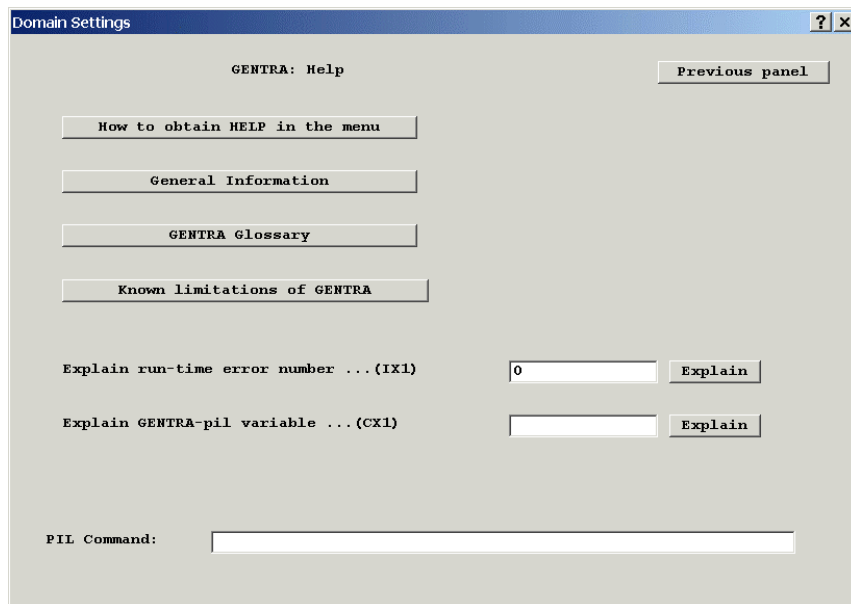


Figure 2.3: Help and information

The options in this panel are explained below.

- **How to obtain help in the menu.** Help in the GENTRA menu is available at two levels:
 - 1 Help on each menu option can be obtained as explained in Section 2.2.4 above.

2 Help items on special topics are available as choices from the menu. For instance, all the options in the current menu panel are informative ones.

- **General information.** Choose this option to obtain basic information on the use of the GENTRA Input Menu. (The information contained in this menu entry is covered by several sections in this Guide.)
- **GENTRA Glossary.** This entry contains an explanation of the terms used in GENTRA and its documentation.

The GENTRA Glossary has been included in this Guide as Appendix H.

- **Known limitations of GENTRA.** This entry contains a list of the limitations of GENTRA which are known to the GENTRA Development Team. The list is not intended to be exhaustive; but the main limitations are presented and, where possible, alternatives are suggested.

The information contained in this entry is listed in this Guide as Appendix E

- **Explain run-time error number.** GENTRA-EARTH will trap, at run time, a large number of error conditions, and will issue a message to inform the user. The message contains an error number and a short explanation of the error. After entering an error number and clicking **Explain**; a fuller explanation of the error and (if appropriate) avoidance instructions will be provided for that error.

GENTRA errors are classified into:-

Warnings (with numbers between 001 and 299), which do not abort the program but reset some of the user-supplied parameters, that are detected to be inconsistent;

Fatal errors (with numbers between 300 and 599), which abort the program;

Internal errors (with numbers between 600 and 899), which should be referred to CHAM.

By default, all the error messages are written to the screen, but you can change this in the GENIUS subroutine. Section 5.3 below provides details.

- **Explain PIL Variable.** As an alternative to the menu, users can also specify the GENTRA settings using a subset of PIL variables (see Chapter 3 for details). Enter a variable name then click **Explain**. Concise reference information will be displayed.

The information provided is summarised in Appendix B of this Guide.

- **Previous panel.** This option returns the user to the previous menu panel. This button is common to all the GENTRA menu panels.

* If you are following the worked example, you can now explore all these sources of information if you so wish, and return to the GENTRA main menu.

2.5 Particle type

The option **Particle type** of the Main Menu (figure 2.2), allows you to specify the type of particle (e.g., vaporising droplet, melting particle, etc); and the physics of the particle type (e.g., drag law, specific heat, buoyancy effects, turbulent dispersion).

When you choose this option, the menu panel in figure 2.4 is produced. The options in the panel are now dealt with in successive subsections.

* Click on **Particle type** now.

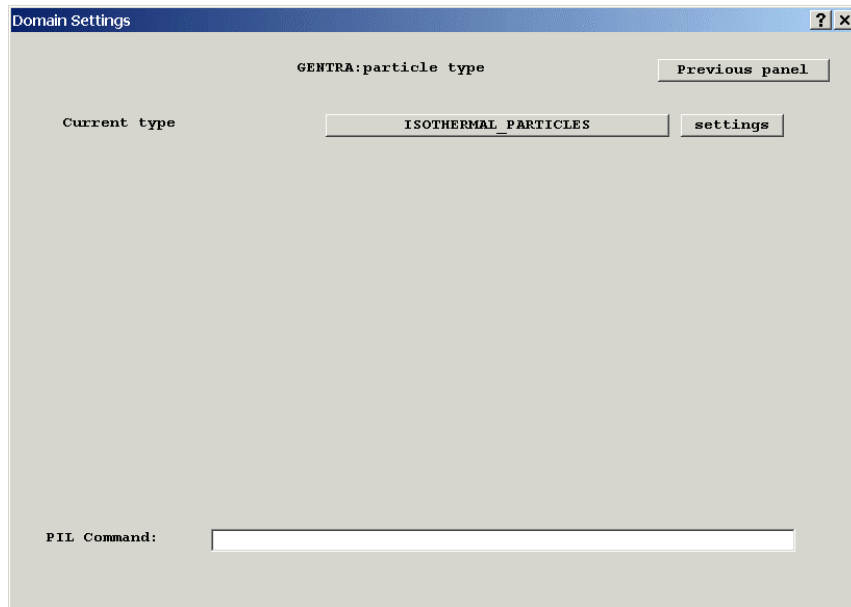


Figure 2.4: Particle type

The particle type to be simulated is selected by clicking on the name of the particle type, which by default is **Isothermal Particles**. This displays a list of available particle types, shown in Figure 2.5. The **settings** button allows the specification of the physics and data of the chosen particle type. Finally, there is an option to return to the previous menu.

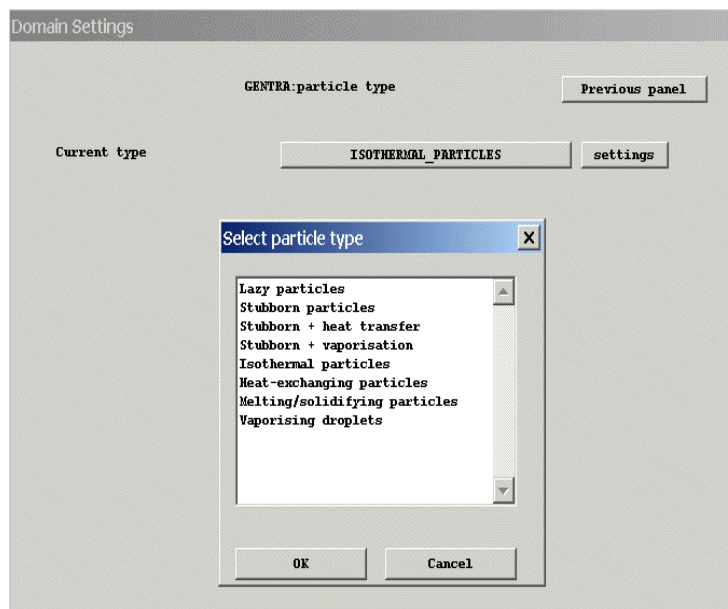


Figure 2.5: Particle type selection

- * For the worked example, the isothermal particle type should be selected. The number of inputs for this particle type is small, but permits the typical features of all panels to be examined.
- **Lazy particles** ($V_{\text{part}} = V_{\text{fluid}}$). “Lazy” particles do not have a velocity of their own, but share, at each point, the continuous-phase velocity. They therefore behave like tracers.

Lazy particles do not have a size or a temperature, and cannot undergo any physical process (such as solidification, or vaporisation) though turbulent dispersion is permitted. Lazy particles have no effect on the continuous-phase solution.

On hitting a wall or obstacle, the lazy particle will be removed from the domain.

- **Stubborn particles** ($V_{\text{part}} = \text{const}$). “Stubborn” particles have a constant velocity, independent of the continuous-phase conditions. They therefore behave like “beams” or “rays”.

Stubborn particles do not have a size or a temperature, and cannot undergo any physical process (such as dispersion by turbulence, or solidification, or vaporisation). They do not exchange momentum with the continuous phase.

On hitting a wall or obstacle, the stubborn particle will be removed from the domain.

- **Stubborn + heat transfer** ($V_{\text{part}} = \text{const}$). “Stubborn + heat transfer” particles behave like “Stubborn” particles, except that they can exchange heat with the continuous phase.
- **Stubborn + vaporisation** ($V_{\text{part}} = \text{const}$). “Stubborn + vaporisation” particles behave like “Stubborn” particles, except that they can exchange heat and mass with the continuous phase.
- **Isothermal particles**. Isothermal particles are modelled by Lagrangian equations for the particle position and velocity, but not for the particle temperature or size. Therefore, this type of particle should be selected when no exchange of heat or mass between the continuous and the disperse phase is to be considered.

On hitting an obstacle, an isothermal particle can either be removed from the domain or bounced with a user-supplied restitution-coefficient.

- **Heat-exchanging particles**. Transfer of momentum and enthalpy between the continuous and disperse phases is accounted for when heat-exchanging particles are employed. The particles are modelled by Lagrangian equations for the particle position, velocity and temperature.
- **Melting/solidifying particles**. Melting/solidifying particles are modelled in a similar way to heat-exchanging particles. However, the Lagrangian equation for the particle temperature includes the effects of solid-liquid and liquid-solid phase change, and the particle diameter is determined as a function of the proportion of the solid and liquid phases present.
- **Vaporising droplets**. Vaporising droplets are modelled by Lagrangian equations for the particle position, velocity, temperature and mass. Exchange of momentum, enthalpy and mass between the disperse and continuous phases is included.

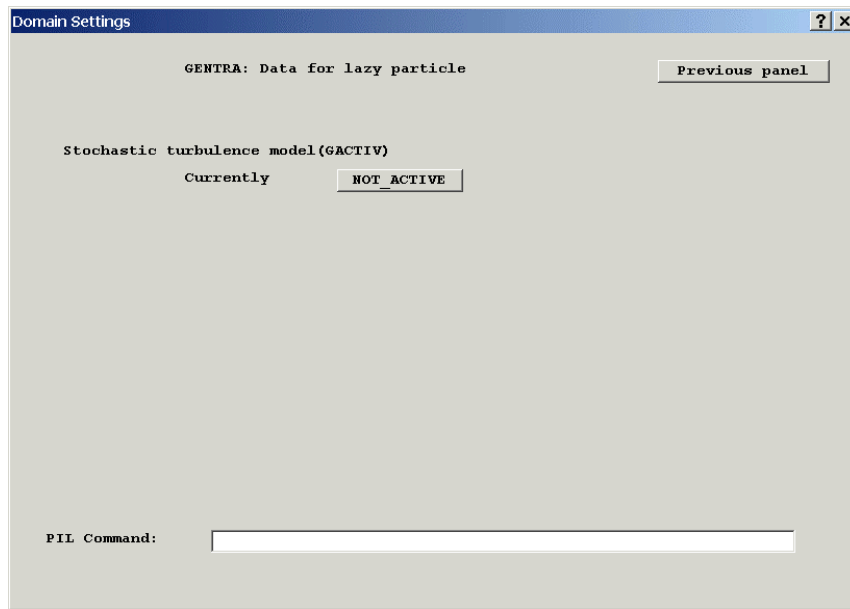
The choice of a particle type should normally be your first action when using the GENTRA Menu, as some of the menu options (e.g., those concerning physical data or particle-obstacle interaction) will depend on the type of particle.

2.6 Physics of current particle type

The **settings** button on the Particle type panel enables the user to specify values for the particle physics (such as drag law, Nusselt numbers, specific heat, buoyancy effects, turbulent dispersion).

The data items to be supplied are dependent on the particle type selected in the previous menu panel. The user is therefore advised to select the correct particle type before visiting this data section.

The following subsections describe the data panels for each of the available particle types.

(a) Data for lazy particles**Figure 2.6: Data for lazy particles**

The only data required for lazy particles concerns the use of the stochastic turbulence model for particle dispersion.

GENTRA has a built-in model that simulates the effect of the turbulent fluctuations of the continuous-phase velocity on the dispersion of particles.

The selection of the option **Stochastic turbulence model** in the Particle physics menu (figure 2.6) will alternately activate/deactivate this feature.

- * Try this now by clicking **not_active**; the stochastic turbulence model will be activated. Click **active**, and it will be deactivated again. Then return to the GENTRA main menu panel by choosing **Previous panel**.

Note that, for the stochastic model to be available, the k- ϵ model of turbulence must be used. GENTRA-EARTH will automatically deactivate it if KE and/or EP are not SOLVED for or, at least, STORED.

When the stochastic turbulence model is selected, the particle trajectories will be calculated from the sum of the mean continuous-phase velocity and an instantaneous turbulent velocity fluctuation determined from the local turbulence conditions.

(b) Data for stubborn particles

No additional data is required for this particle type.

(c) Data for isothermal particles

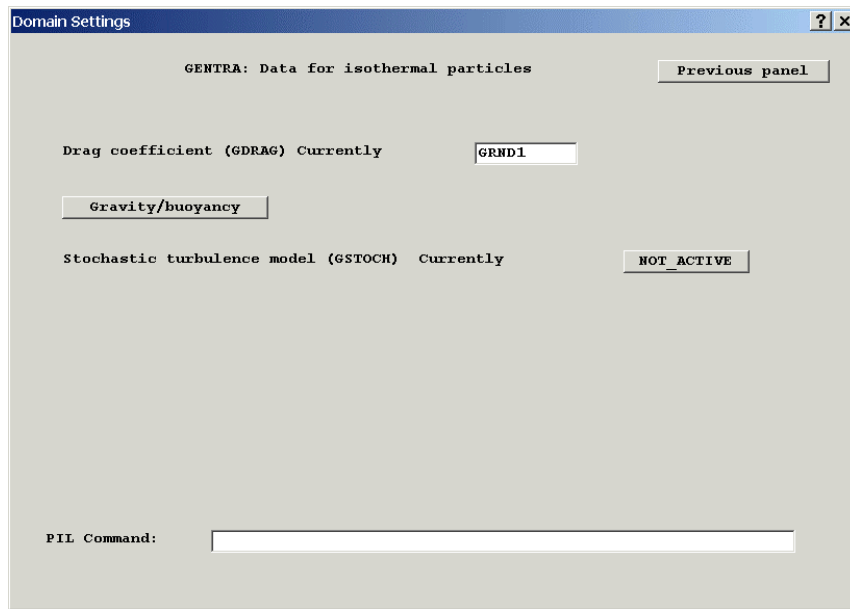


Figure 2.7: Data for isothermal particles

The **drag coefficient** (which is responsible for the exchange of momentum between the disperse and the continuous phase) can be specified in one of two ways:-

- If a constant is used, the drag coefficient will be taken as equal to that constant.
- Special flags can be used to specify laws. The built-in laws and associated flags are as follows:

Flag	Law
GRND1 (or -10120.)	Solid spheres

(See Chapter 6 of this Guide for mathematical expressions)

You can introduce your own law in Section 1 of GPROPS (see Chapter 5 for details). Recompilation and re-linking of EARTH is needed after the modification of GPROPS.

- * The built-in law will suffice for the worked example. However, you can enter other values, then enter GRND1 again for the sake of practice. Then return to the previous panel by clicking **Previous panel**.

The **gravity/buoyancy** forces option enables the user to activate gravity forces for the particles, and to include buoyancy and pressure gradient effects. The option brings up the menu panel displayed in figure 2.8.

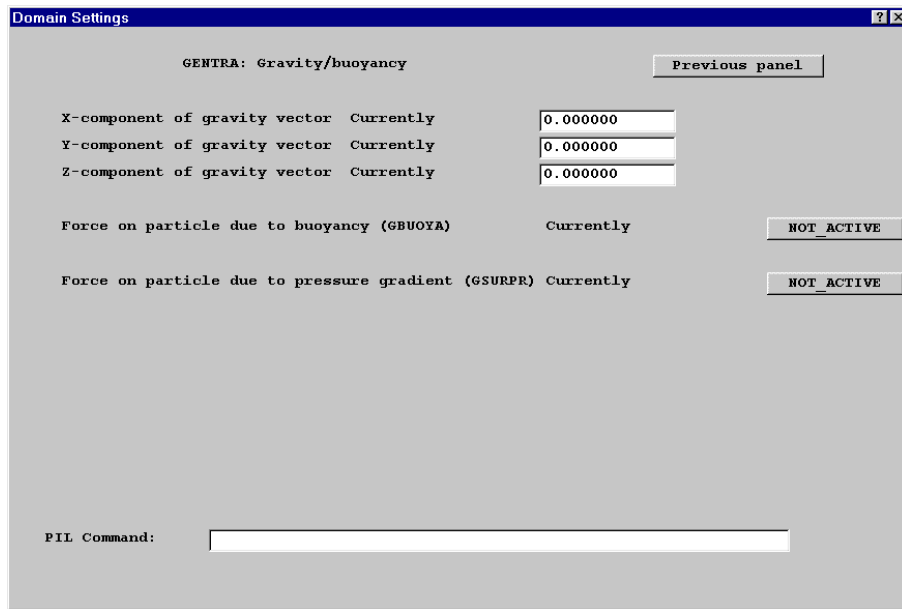


Figure 2.8: Gravity/buoyancy

- **X-, Y-, Z-component of gravity vector.** Use these options to specify the three components of the gravitational acceleration acting on the particles. The components of the gravitational acceleration must be supplied in the GENTRA Cartesian System, regardless of the co-ordinate system being employed for the continuous phase. (See entry in the GENTRA glossary for a description of the GENTRA Cartesian System).

* Enter 9.8 for **Z-component of gravity vector** to specify an acceleration of 9.8 m/s^2 acting along the z axis.

- **Force on particle due to buoyancy.** This option activates/deactivates the buoyancy formulation. When active, it introduces a multiplicative factor $(1 - \rho_c/\rho_p)$ in the gravity term of the particle momentum equation. See Section 6.3.2 for details.
- **Force on particle due to pressure gradient.** This option activates/deactivates the pressure gradient term in the particle momentum equation (see Section 6.3.2 for details).

If P1 includes the hydrostatic pressure, then the user selects:

- pressure gradient term to active** and **buoyancy term to not_active**, to include all the fluid forces on the particle; or
- pressure gradient term to not_active** and the **buoyancy term to active**, to include only buoyancy.

If P1 excludes the hydrostatic pressure (reduced pressure formulation), then the user should select:

- pressure gradient term to active** and **buoyancy term to active**, to include all fluid forces on the particle;
- pressure gradient term to not_active** and **buoyancy term to active**, to include only buoyancy.

(d) Data for heat-exchanging particles

Domain Settings

GENTRA: Data for heat-exchanging particle

Previous panel

Drag coefficient (GDRAG) GRND1

Thermal conductivity of continuous phase (GKONC) 0.026300

Nusselt number (GNUSS) GRND1

Cp of particle (GCPLIQ) 4131.800

Cp of continuous phase (GCPCON) 1007.000

Gravity/buoyancy

Stochastic turbulence model (gactiv) Currently NOT_ACTIVE

FIL Command:

Figure 2.9: Data for heat-exchanging particles

The selection of drag coefficient is identical to that for the case of isothermal particles; see subsection (c) above for a complete explanation.

- Thermal conductivity of continuous phase.** This option must be selected. A value of 0.0263 W/m/k is given as the default, corresponding to air at STP. If the user wishes to include his own temperature-dependent function for the thermal conductivity of the continuous phase, he should do the following:
 1. Replace the constant value in the menu with a GRND number (i.e. GRND1).
 2. Modify function routine GPROPS in the file GENTRA.FTN by adding coding in the relevant section. For this case, the coding should be added in the section commencing "GROUND1", and in the subsection commencing "3 Thermal Conductivity of the continuous phase". Coding relating the thermal conductivity (GPROPS) to the continuous-phase temperature (PARAMT) should then be inserted.
 3. Before running EARTH, the GENTRA file will have to be recompiled and the EARTH executable relinked.
- The **Nusselt number** is defaulted to GRND1. This implies that the Nusselt number will be calculated from the correlation of equation (6.8); other correlations may be included in GPROPS following a procedure similar to that outlined above for the setting of the continuous-phase thermal conductivity. Alternatively, the Nusselt number may immediately be specified as a constant during this menu session.
- The **specific heat capacity of the particle** is defaulted to 4131.8 J/kg/k, which is representative of liquid water. Other constant values can be substituted for this or it can be replaced by a particle-temperature-dependent function in GPROPS.
- A constant value of 1007 J/kg/k is provided as the default value for the **specific heat capacity of the continuous phase**, this being the value for air at STP. The constant value can be altered during the menu session, or a temperature-dependent function can be implemented using the techniques mentioned above.

Gravity and buoyancy/pressure gradient effects and turbulent dispersion can be included; the reader is referred to the entries in sub-sections (c) and (a) above, for an explanation.

(e) Data for melting/solidifying particles

Domain Settings

GENTRA: Data for melt/solidif. particle

Previous panel

Drag coefficient (GDRA) GRND1

Thermal conductivity of continuous phase (GKONC) 0.026300

Nusselt number (GNUSS) GRND1

Cp of liquid (GCPLIQ) 4131.800

Cp of solid (GCPSOL) 4131.800

Cp of continuous phase (GCPCON) 1007.000

Latent heat of solidification (GLHEAS) 333500.0

Index for solid-frac formula (GSOLIN) 1.000000

Solidus temperature (GSOLST) 273.1500

Liquidus temperature (GLIQST) 273.1500

Gravity/buoyancy

Stochastic turbulence model (gactiv) Currently NOT_ACTIV E

PIL Command:

Figure 2.10: Data for melting/solidifying particles

The data required for melting/solidifying particles is as follows:

- **Drag coefficient** (see Subsection (c) for explanation).
- **Thermal conductivity of continuous phase.** The default value of 0.0263 is for air at STP.
- **Nusselt number** (see Subsection (d) for explanation).
- **Cp of liquid** phase of the melting/solidifying particle. The value of 4131.8 is representative of water.
- **Cp of solid** phase of the melting/solidifying particle.
- **Cp of continuous phase.**
- **Latent heat of solidification.** The default value of 3.335E+05 is for the formation of water ice. If the specific heat capacities of the liquid and solid phases were not identical, and if the change of phase was not isothermal, the latent heat of solidification would be temperature dependent, and a function would be required for it in GPROPS. Further explanation of this is provided in Section 6.3.4.
- **Index for solid fraction formula** (equation (6.15)). For the case of isothermal phase change, this variable is not employed.
- **Solidus temperature** of particle. The maximum temperature at which the particle is completely in the solid phase. The default value is for water.
- **Liquidus temperature** of particle. The minimum temperature at which the particle is completely in the liquid phase. The default value is for water.
- **Gravity/buoyancy/pressure forces.** (See Subsection (c) above for this option).
- **Stochastic turbulence model.** (See Subsection (a) above for details on this option).

The constant values which appear in this menu can be replaced with functions set in function routine GPROPS, according to the method described in Subsection (c) above.

(f) **Data for vaporising droplets**

The screenshot shows a window titled 'Domain Settings' with a sub-header 'GENTRA: Data for vaporising droplets'. A 'Previous panel' button is in the top right. The parameters and their values are as follows:

Drag coefficient (GDRA)	GRND1
Nusselt number (GNUSS)	GRND1
Cp of continuous phase (GCPCON)	1007.000
Cp of Vapour (GCPVAP)	GRND1
Cp of particle (GCPLIQ)	4131.800
Latent heat of evaporation (GLATVP)	GRND1
Particle liquid saturation enthalpy (GHLIQD)	GRND1
Saturation temperature (GVAPST)	GRND1
Saturation pressure (GSTPRE)	GRND1
Thermal conductivity of continuous phase (GKONC)	0.026300
Thermal conductivity of Vapour (GKONV)	GRND1
Mol. Weight of continuous phase (GMWCON)	28.90000
Mol. Weight of particle phase (GMWVAP)	18.00000
Minimum particle diameter (GDTRCT)	0.000000

Below the table is a 'Gravity/buoyancy' button. At the bottom, there is a 'PIL Command:' label followed by a text input field, and 'Page Dn' and 'Line Dn' buttons.

Figure 2.11: Data for vaporising droplets

- **Drag coefficient.** (See Subsection (c) for explanation.)
- **Nusselt number.** (See Subsection (d) for explanation.)
- **Cp of Continuous phase.** The default value of 1007 is for air at STP.
- **Cp of Vapour.** The value of CV is defaulted to GRND1, which directs control to GPROPS where a temperature-dependent property is specified.
- **Cp of Particle.** The default value of 4131.8 is for water.
- **Latent heat of evaporation.** A saturation-temperature-dependent function for the latent heat of evaporation is provided as the default value, GRND1. The function is for water vapour, and is derived from curve-fits on steam tables.
- **Particle liquid saturation enthalpy.** The default value of GRND1 produces a temperature-dependent function for the liquid saturation enthalpy of water, based on curve fits from steam tables.
- **Saturation temperature** of vapour. The default value of GRND1 provides a function for the saturation temperature of water vapour as a function of pressure.
- **Saturation pressure** of vapour. The default value of GRND1 provides the temperature-dependent vapour pressure correlation of Bain (1964).
- **Thermal conductivity of continuous phase.** The default value of 0.0263 is for air at STP.
- **Thermal conductivity of vapour.** The default value of GRND1 provides a temperature-dependent function for water vapour based on curve-fits to steam tables.
- **Molecular weight of continuous-phase,** defaulted to air (28.9).

- **Molecular weight of particle phase**, defaulted to water (18.0).
- **Minimum particle diameter**. The minimum size of particle below which the particle is assumed to have completely evaporated.
- **Gravity/buoyancy/pressure forces**. (See Subsection (c) above for details on this option.)
- **Stochastic turbulence model**. (See Subsection (a) above for details on this option.) This option appears on the next panel, reached by clicking **Page down**, or **Line down**.

The constant values, which appear in this menu, can be replaced with functions set in function routine GPROPS, according to the method described in Subsection (c) above.

2.7 Boundary conditions for particles

The **Boundary conditions** button in the Main Menu panel (figure 2.2) is used to specify the boundary conditions for the particles. Boundary conditions fall into the following categories:-

- **Inlets**: The injection position and the particle properties (eg, velocities, diameter, temperature, etc) at the inlet must be given;
- **Exits**: The boundary regions at which the particles can leave the domain must be specified;
- **Symmetry surfaces**: The location of the symmetry surfaces (at which particles must be reflected) must be supplied;
- **Wall/obstacles**: The behaviour of the particle following the collision with a wall or obstacle is selected from a range of choices (such as bouncing, sticking or flash vaporisation).

* Click on **Boundary conditions** to bring up the Boundary conditions panel.

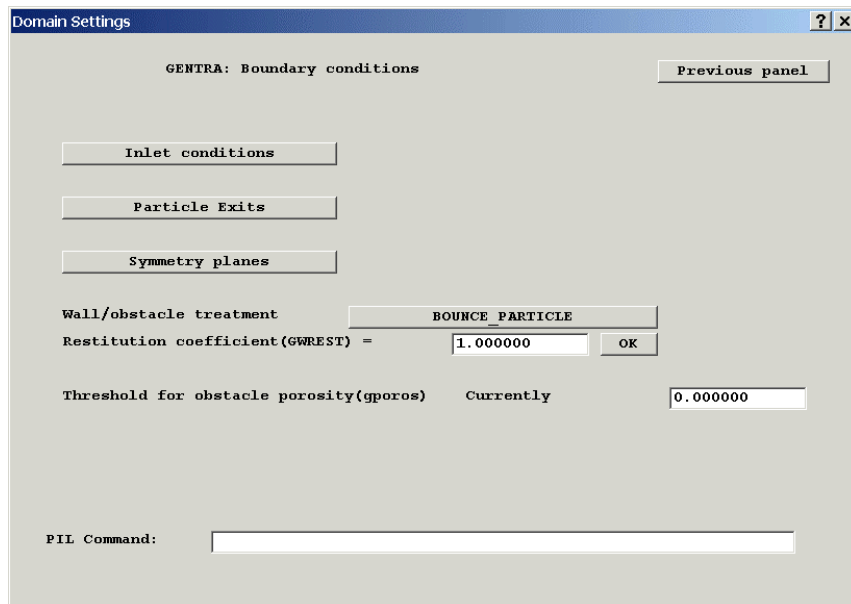


Figure 2.12: Boundary conditions for particles

The options in the Boundary conditions panel (shown in figure 2.12) are dealt with in subsequent subsections.

2.7.1 Inlet conditions

The Inlet conditions option of the Boundary conditions panel produces the panel in figure 2.13.

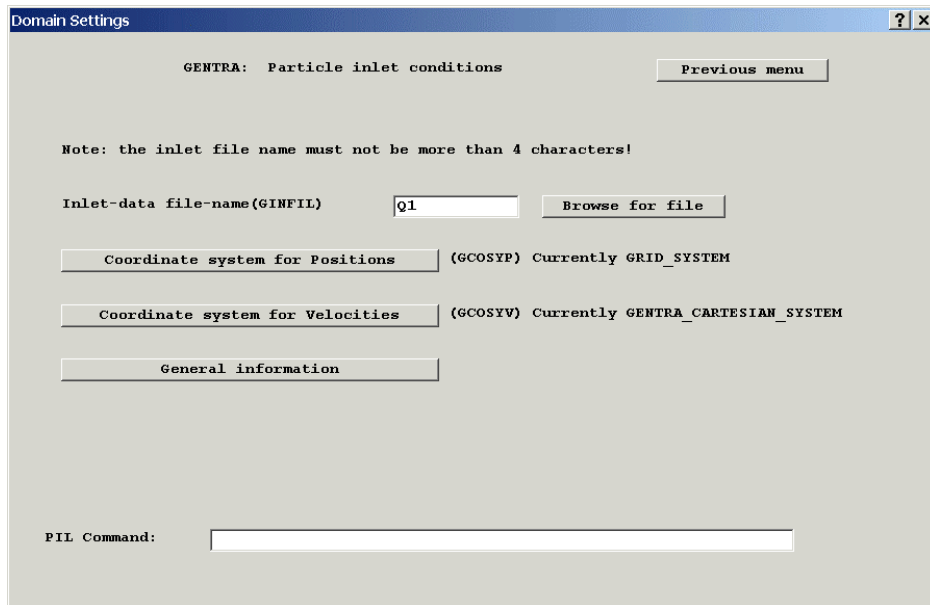


Figure 2.13 Particle inlet conditions

- **Inlet-data file-name.** The inlet data in GENTRA is specified in a table located in an **inlet-data file**. The user can select the name of the inlet-data file through this option (the maximum length of the file name is 4 characters). Further information on the contents and format of the inlet data can be found at the end of this sub-section.

* The default file-name, Q1, will be used for the worked example.

- **Coordinate system for Positions.** (Option not available in the present version of GENTRA.)

This option allows the specification of inlet co-ordinates in the inlet file in either the GENTRA Cartesian system (see glossary entry for a definition) or in the grid system. The distinction is only relevant to cylindrical-polar grids, since in Cartesian and BFC the GENTRA Cartesian system and the grid system coincide.

At present, the particle positions must be specified in the grid co-ordinate system. Thus for cylindrical-polar grids, the co-ordinates are specified as θ , r , z . The alignment between the Cartesian and polar grid systems is explained in Appendix H.

- **Coordinate system for Velocities** (Option not available in the present version of GENTRA.)

This option allows the specification of inlet velocities in the inlet file in either the GENTRA Cartesian system (see glossary entry for a definition) or in the grid system. The distinction is only relevant to cylindrical-polar and BFC grids, since in Cartesian grids the velocity components in the GENTRA Cartesian system and in the grid system are the same.

At present, all inlet velocities must be specified in the Cartesian co-ordinate system, in the order U_{crt} , V_{crt} , W_{crt} , where these represent the velocity components in the Cartesian X , y and Z directions respectively. For cylindrical-polar grids, the order of specification is V_{crt} , U_{crt} and W_{crt} .

2.7.1.1 Format and contents of the inlet-data table

Inlet data In the inlet-data table, each parcel of particles has a data line; the data required is case-dependent. For the user's guidance, the GENTRA menu will generate, as a comment in the resulting Q1 file, a suitable heading for the inlet table.

The contents of the inlet table are also provided below for the different particle types.

Particle	Properties required
Lazy	POSTN
Stubborn	POSTN VELOC
Isothermal	POSTN VELOC DIAM DENSTY FRATE (NUMB)
Heat-exchanging	POSTN VELOC DIAM DENSTY FRATE TEMP (NUMB)
Melt/solidifying	POSTN VELOC DIAM LIQDEN FRATE TEMP SOLDEN (NUMB)
Vaporising	POSTN VELOC DIAM DENSTY FRATE TEMP (NUMB)

In the table above,

- POSTN is the parcel inlet-position, in the co-ordinate system selected by the user (for one- or two-dimensional cases, no co-ordinates are needed for the dimensions for which the number of cells are one);
- VELOC is the parcel inlet velocity-components, in the co-ordinate system selected by the user (for one- or two-dimensional cases, no components are needed for the dimensions in which the number of cells are one);
- DIAM is the particle diameter;
- DENSTY is the density of the particle; LIQDEN is the density of the liquid phase in solidifying particles (Units: kg/m³);
- FRATE is the mass-flow rate of particles (Units: kg/s)
- TEMP is the particle temperature (in K);
- SOLDEN is, for melting/solidifying particles, the solid-phase density.
- (NUMB) is an optional parameter, indicating the number of parcels of the given characteristics to be released from that position. When the stochastic turbulence model is active, GENTRA will track every parcel separately. When the stochastic turbulence model is inactive, GENTRA will simply multiply the mass-flow rate by the number of parcels and track a single parcel. When the NUMB data-item is missing, one parcel is assumed.
- **Comments** Those lines in the inlet table containing, in any position, an asterisk (*) are treated as comments. The table heading can be inserted in this way in the data file. Blank lines are also ignored.
- **Line length** The maximum length of an inlet-table line is 132 characters.
- **Number formatting** The formatting of the numbers in the inlet table is free, but items of data must be separated with spaces (), commas (,) or semi-colons (;).
- **Error trapping** GENTRA will skip those data lines that contain invalid characters (such as letter O instead of number zero), or that have a different number of data items to that which is required.

2.7.1.2 Q1 file as input file

By setting the inlet-data file-name to Q1 (the default), GENTRA will expect the inlet-data table to be in the Q1 file. All of the format rules for the inlet-data table (listed above) apply to the Q1 file. In addition, when the inlet data-table is in the Q1 file, the following practices must be observed:-

- Inlet-data lines must be PIL comments; i.e., they must not start in the first or second column of the Q1 file, since they would be treated as commands by the SATELLITE.
- The inlet-data table must be preceded and terminated by two special marks (also inserted as PIL comments). These marks are: <GENTRA-INLET-DATA> and <END-GENTRA-INLET> respectively.
- **WARNING:** The maximum length of the inlet-data line is 132 characters. However, users are advised that the maximum length of a Q1-file line for the SATELLITE is 68 characters; if the SATELLITE is run after the inlet data has been inserted, and, following instructions from the user, the Q1 file is re-written, all the data items in columns 68 onwards will be lost.

The inlet-data table can be located anywhere in the Q1 file, and is normally written using a system file-editor after the menu session.

Note: GENTRA can **generally** cope with inlets lying **exactly** on the boundaries of the domain or on the grid pole; it is nevertheless a good practice to offset the inlet position by a small distance (e.g., 10^{-4} m).

* In this worked example, we will write the data table after finishing the menu session

2.7.1.3 Editing the File Containing the Input Data Table

In the VR-Environment, the file containing the inlet data table can be opened for editing by clicking on '**File**', '**Open file for editing**'.

If the inlet data table is in Q1, select '**Q1**', and then click '**Yes**' to save the current settings to Q1. After editing the inlet data table, save the file and exit the editor. Click '**Yes**' to reload the Q1 into VR-Editor, otherwise the new data will be lost.

To open any other file, select '**Any file**', then open it from within the editor.

The editor used can be selected from '**Options**', '**Text file editor**'.

2.7.2 Exits

Particle exits in GENTRA are represented through PATCH commands. Particle exit-PATCHes must have names beginning with GX, and be of an area type (ie, EAST, WEST, NORTH, SOUTH, HIGH, LOW).

In the VR Environment, all Inlet and Outlet objects act as GENTRA exits by default – the PATCHes they create all have names starting with GX. This behaviour can be altered by the '**Acts as GENTRA exit**' buttons at the foot of the Inlet and Outlet object attribute dialogs. Note that these buttons only appear once GENTRA is active. The buttons can be seen in Figure 2.14.

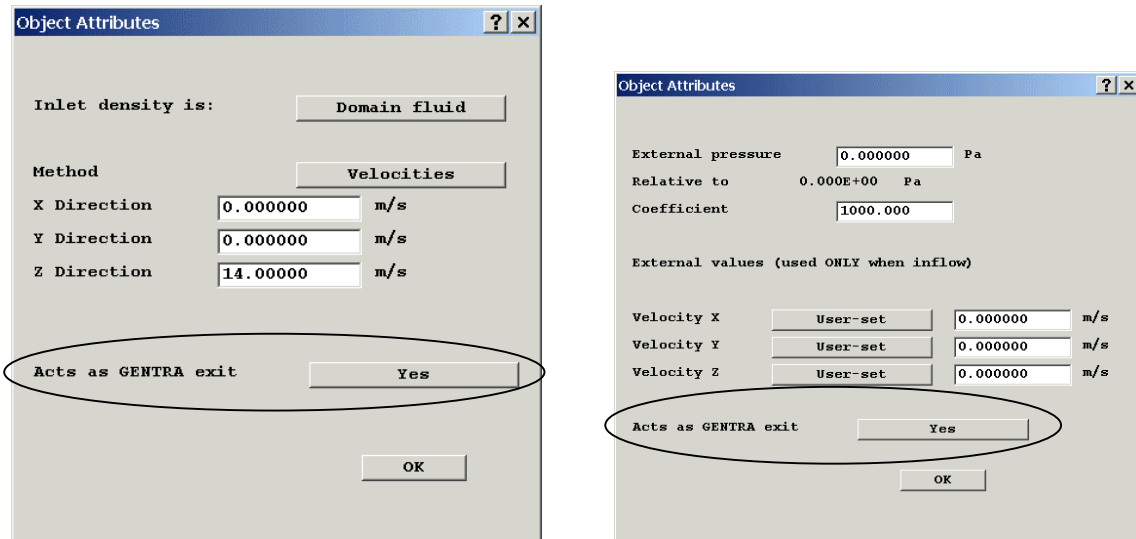


Figure 2.14: Inlet and Outlet attribute dialogs

To create an exit where only particles can leave the domain, set the coefficient for the pressure to zero in the Outlet attributes dialog. This will prevent the continuous phase from passing through.

2.7.3 Symmetry surfaces

The treatment for particles at an axis/surface of symmetry is always reflection (i.e., bouncing with a restitution coefficient of 1), regardless of the wall treatment selected for the problem.

GENTRA will automatically detect symmetry axes in the following two circumstances:

- In 2D cylindrical-polar cases, and 3D cylindrical-polar cases in which the domain covers less than 2π radians in the circumferential direction, the grid pole is treated as an axis of symmetry.
- In “wedge-like” 2D BFC domains (in which one of the domain sides collapses to a line), the edge of the wedge is treated as a symmetry axis.

In all other cases, axes/surfaces of symmetry must be declared by the user, so that GENTRA can act appropriately when a particle hits the axis/surface.

Symmetry surfaces in GENTRA are represented through PATCH commands whose PATCH name starts with GS. Each symmetry PATCH has also an associated PATCH type. This indicates on which face of the cells covered by the PATCH the symmetry surface is. The PATCH type can be EAST, WEST, NORTH, SOUTH, HIGH or LOW.

In the VR Environment, GENTRA symmetry surfaces are created by making a new object, with type **GENTRA_SYMMETRY**. This object type is only available when GENTRA is active. The PATCH created by such an object will have a name starting with GS, and will be of the correct type.

- * The grid in the worked example is of the “wedge-like” kind; the axis will therefore be automatically detected by GENTRA.

2.7.4 Wall/obstacle treatment

The option Wall/obstacle treatment in the Boundary conditions panel (figure 2.12) specifies how the particle interacts with walls and obstacles (e.g., bouncing, sticking, removal).

See the GENTRA Glossary for a definition of wall/obstacle.

The options available depend on the type of particle; the user is therefore advised to set the particle type before visiting this menu. (The panel in figure 2.15 shows all of the possible treatments.)

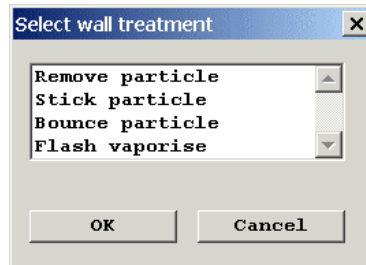


Figure 2.15: Wall/obstacle treatment

The menu Wall/obstacle treatment has, in the general case, the following options (figure 2.15):

- **Remove particle** from domain. On hitting a wall or obstacle, the particle will be removed from the domain (ie, the tracking algorithm will abandon the particle and move on to the next one).
- **Stick particle** to the wall. On hitting a wall or obstacle, the particle will remain stationary, but it will still undergo heat- and mass-transfer processes if the particle type allows for these.

(Note that REMOVE PARTICLE and STICK PARTICLE have the same effect for isothermal particles.)

- **Bounce particle** off the wall. On hitting a wall or obstacle, the particle will be bounced. A restitution coefficient must be provided. The restitution coefficient is the absolute value of the ratio between the velocity component normal to the wall before and after the contact. The restitution coefficient must be greater than 0 and less than or equal to 1.

See Section 6.6.2 for more information on bouncing.

* Choose **Bounce** and set a restitution coefficient of 0.75 for the worked example. Then return to the previous panel.

- **Flash vaporisation.** On hitting a wall or obstacle, the particle will be vaporised instantly, and all the mass will be transferred to the continuous phase.

This option is available only for VAPORISING DROPLETS.

2.7.5 Threshold for obstacle porosity

This option of the Boundary conditions panel (figure 2.12) allows the user to set the level of porosity that will be considered by GENTRA to constitute an obstacle for the particles.

For instance, a value of 0.75 will indicate that cells and cell faces with porosities between 0.0 and 0.75 will be taken as obstacles for the particulate phase.

Only values between 0 and 0.999 are accepted.

2.8 Numerical controls

The option **Numerical controls** of the main menu (figure 2.2) allows the user to control the solution procedure for the particulate phase. Users can, for instance:-

- Delay the first call to GENTRA until the continuous-phase flow-field has settled;
- Specify a frequency for calls to GENTRA;
- Set timeout limits for the particle flights;
- Apply relaxation to the interphase sources;

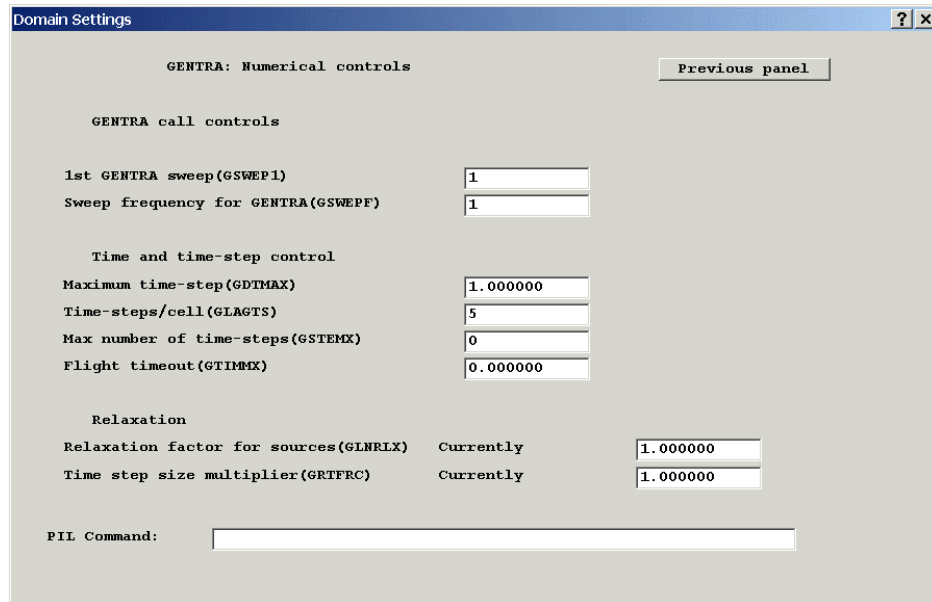


Figure 2.16: Numerical controls

- **1st GENTRA sweep.** This option allows the user to set the first EARTH sweep at which GENTRA will be called.

It is often a good practice to start the particle tracking when the continuous-phase field is developed. The selection of values greater than 1 for this option will have that effect.

This option can also be used to switch off the particle tracking by setting a value greater than the number of PHOENICS sweep (LSWEEP). If GENTRA is deactivated in this fashion, all the GENTRA settings will be retained in the Q1. It will be possible to turn GENTRA on again later. If GENTRA is turned off from the Models panel, all GENTRA settings are cleared. To turn GENTRA back on would involve re-setting all the non-default values.

* The number of PHOENICS sweeps for the example is LSWEEP=200; choose 190 as the first GENTRA sweep.

- **Sweep frequency for GENTRA.** This option sets the frequency (in terms of EARTH sweeps) for calls to GENTRA. For instance, a value of 5 will cause the particle tracking to be effected for those sweeps whose index is a multiple of 5, and greater than or equal to the user-specified first-GENTRA-sweep (see option 1 in this menu).

Values greater than 1 are recommended, in conjunction with source relaxation, for high particle loadings; for the continuous phase is then able to "absorb" the interphase sources before the next call to GENTRA.

* Since the particle loading will not be a high one in the worked example, the default value will suffice.

- **Maximum time-step** This option allows the user to specify a maximum Lagrangian time-step, which will not be exceeded by GENTRA. (Note, however, that this time step may be **reduced** by GENTRA according to particle position and flow conditions.)
- **Time-steps/cell.** This option sets the **approximate** number of integration steps for each particle within each cell. A value of 5 is recommended. Note that this number can be increased (and occasionally reduced) by GENTRA according to flow conditions. (See Section 6.5.1)
- **Max number of time-steps.** This option allows the user to specify a maximum number of Lagrangian time-steps. If this limit is reached during the tracking of a particle, the particle is abandoned, a timeout message is issued and GENTRA moves on to the next particle.

This device can, for instance, avoid large computing times arising from very small time-steps.

The step number n can be positive, negative or zero:-

- $n > 0$ abandons the tracking after n time-steps;
- $n = 0$ deactivates this timeout device;
- $n < 0$ indicates that the time-step limit is to be applied in each cell (ie, the timeout counter is reset when the particle enters a new cell).

* Enter -100 for the worked example.

- **Flight timeout.** This option allows the user to specify a time limit for the tracking. If this limit is reached during the tracking of a particle, the particle is abandoned, a timeout message is issued and GENTRA moves on to the next particle.

This device can avoid large computing times arising, for instance, from particles being trapped in recirculation regions.

The timeout value r can be positive, negative or zero:-

- $r > 0$ abandons the tracking after the particle has been tracked for r seconds;
- $r = 0$ deactivates this timeout device;
- $r < 0$ indicates that the timeout limit is to be applied in each cell (i.e., the timeout counter is reset when the particle enters a new cell).

* Enter 10 for the worked example. Since the fluid inlet-velocity is 2.0 m/s, and the domain length in that direction is 2 m, the particles can be expected to have left the domain in that time.

- **Relaxation factor for sources.** This option allows the user to specify a linear-relaxation factor (a real number between 0 and 1) for the sources that account, in the continuous-phase equations, for the transfer of momentum, mass and thermal energy from the particles.

Values between 0 and 1 have the effect of setting the source to be a weighted average of the sources calculated at the current and previous sweeps i.e.:

$$S\phi = \alpha S\phi_n + (\alpha - 1) S\phi_{n-1}.$$

This may be beneficial for the convergence of the continuous-phase solution when the source is changing significantly from sweep to sweep;

- a value of 1 applies no relaxation to the source, (ie only the source calculated at the current sweep is employed); and
- a value of 0 sets the source equal to that employed at the previous sweep (ie the source does not change).

* Set a relaxation factor of 0.7

2.9 Input/Output controls

This is the last option of the Main Menu Panel (figure 2.2), which controls the input and output data flow of GENTRA. When **I/O controls** is selected in the Main Menu Panel, the following panel will appear.

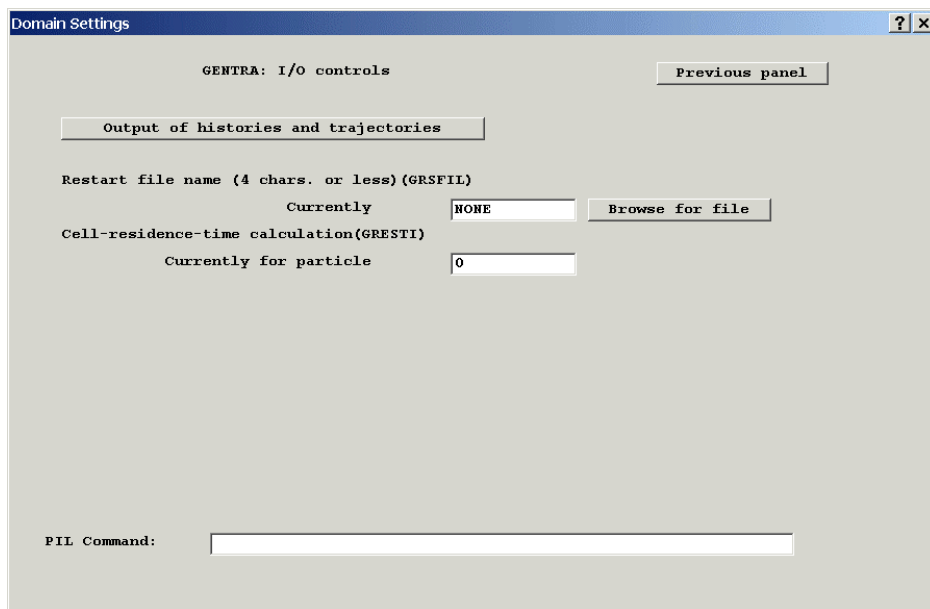


Figure 2.17: Input/Output controls

2.9.1 Output of history and trajectory

Selection of this option produces the panel of figure 2.18.

Domain Settings

GENTRA: History and trajectory file

Previous panel

name of Global history file (4 char.) (GHFILE)

Currently GHIS

output for Individual particle

Frequency (time-steps) for output(GOUTFR)

Currently 1

PIL Command:

Figure 2.18: History and trajectory files

- **name of the Global history file.** Up to 4 characters can be given to the name of the file. Specifying "NONE" results in no global history file being written by the end of the GENTRA EARTH run.

The global history file contains the results for all of the particles that are tracked. It can be post-processed using the UNPACK program to produce individual history and/or trajectory files. Details of the operation of the UNPACK program can be found in Appendix K.

- **Output for Individual particle.** The panel of figure 2.19 will follow if this option is selected.

* We will require individual trajectory files so choose this option.

Domain Settings

GENTRA: Output for individual particle

Previous panel

ID of indiv. History file(GH1STC)

Currently NONE

ID of indiv. Trajectory file(GT1STC)

Currently NONE

First trajectory to write(NGWSTR)

Currently 0

Last trajectory to write(NGWEND)

Currently 0

Interval of writing trajectories(NGWINT)

Currently 1

PIL Command:

Figure 2.19: Output for individual particle

- **ID of Indiv. history file:** the first character for the name of the individual history file.

- **ID of Individ. trajectory file:** the first character for the name of the individual trajectory file.
- **First trajectory to write:** the first track for which an individual history/trajectory file is required.
- **Last trajectory to write:** the last track for which an individual history/trajectory file is required.
- **Interval of writing trajectories** at which the individual history/trajectory file is written between the two tracks selected in the last two options.

* In this worked example, we would like to produce trajectory files for all five particles being tracked. Therefore, input a suitable character with which the file names should commence, say T. We require trajectory files for each of the first five particles, so select the first and last particles as 1 and 5 respectively. Now select Previous panel twice to return to the I/O controls menu panel.

Note that a maximum of 20 trajectory, and 20 history files can be created in this way. Trajectory and history information for **all** particles is held in the global history file (see figure 2.18 and Appendix K).

2.9.2 Restart file name

The name of the GENTRA restart file. Up to 4 characters can be used. This option is not relevant to steady-state cases. In a transient case, it is the name to which GENTRA writes the particle information at the end of the last time step. This can then be used to continue the run.

2.9.3 Cell-residence-time and particle-volume-fraction calculation

This option in the Output control panel selects a particle for which the cell residence-time will be calculated by GENTRA. The particle is identified by the user through the particle number. In addition to the particle number, two special numbers can be used as flags to perform special functions:-

- 0 will deactivate the calculation of residence time;
- 1 will add the residence time of all the particles in each cell.
- 2 will activate the calculation of a "particle volume-fraction" for each cell, representing the fraction of the cell volume occupied by particles. See Section 6.6.4 for additional details.

* Choose, as an example, to compute the residence time for particle number 2. (Remember that you will define the particle inlet data **after** the menu session.)

When choosing a value different from 0, the GENTRA menu will automatically allocate whole-field storage-space for the variable REST through the command STORE(REST). The variable REST will be used by GENTRA to store the cell residence-time; this can be inspected in the printout of that variable in the RESULT file.

The foregoing options are available for steady flows only (STEADY=T), and the particle volume fraction option is not available for lazy particles (GPTYPE=10) because the particle mass is zero.

For unsteady flow (STEADY=F), the particle volume fraction will be calculated for each cell (see section 6.6.4) provided that STORE(PVFR) appears in the Q1 input file.

2.9.4 Particle-mass-concentration calculation

This option in the Output control panel provides for the calculation of the particle mass concentration for each cell (see Section 6.6.5). It can also be activated by setting STORE(PMCO) in the Q1 input file.

2.9.5 Mixture-density calculation

This option in the Output control panel provides for the calculation of the mixture density for each cell (see Section 6.6.6). It can also be activated by setting STORE(RHMX) in the Q1 input file.

2.9.6 Particle-mass-fraction calculation

This option in the Output control panel provides for the calculation of the particle mass fraction for each cell (see Section 6.6.7). It can also be activated by setting STORE(PMFR) in the Q1 input file.

2.10 Ending the GENTRA Menu session

The GENTRA Menu session is ended from the GENTRA Main Menu Panel, shown in figure 2.2 by clicking on **Previous panel**. This returns control to the normal VR Main menu.

- * Choose this option now to finish. Click on 'Top' and 'OK' to quit the VR Main Menu. Now edit the Q1 file and insert, as comments, the inlet data for the particles. The inlet data must be inserted between the marks <GENTRA-INLET-DATA> and <END-GENTRA-INLET> in the Q1 file. Refer to Section 2.7.1.3 above for instructions, and to the Q1 file in Appendix E for an example. Copy the settings from Appendix E.

2.11 The GENTRA Library

GENTRA has a library of ready-to-run examples and tests. To see the contents of the GENTRA Input Library, click on **File, Load from Libraries** on the VR Environment top menu.

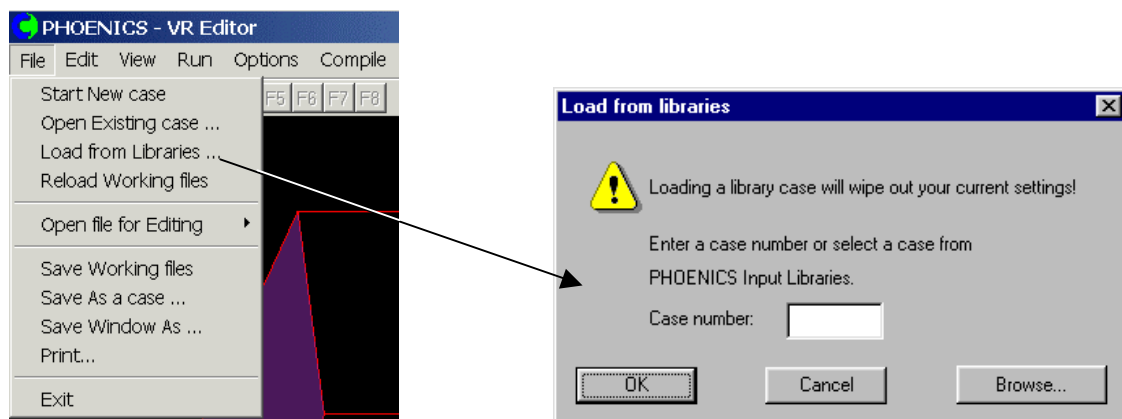


Figure 2.20: Accessing the Libraries

On the library dialog, click on **Browse**, then open the Option Libraries branch of the library tree. The GENTRA libraries are further subdivided as shown in Figure 2.21

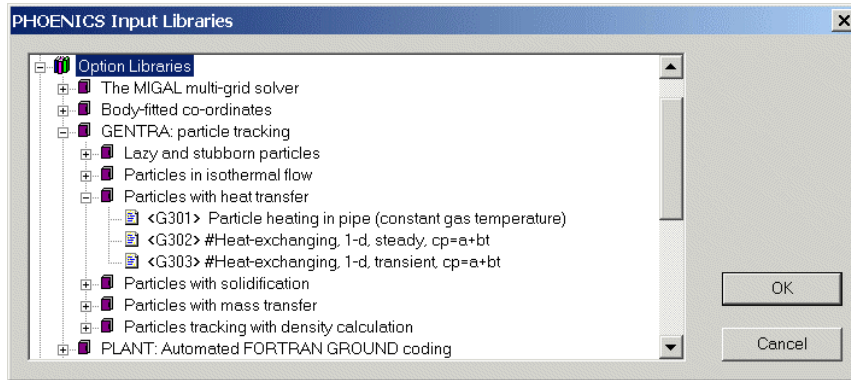


Figure 2.21: The GENTRA Input Library

The contents of the Library are listed as Appendix F of this Guide.

Once the GENTRA Menu session is ended, or a library case has been loaded, you are ready to execute the calculating program EARTH. Chapter 4 explains how to do so. (You can skip Chapter 3, which gives additional details on data input using PIL, if you are a beginner.)

3 Using GENTRA PIL

3.1 Introduction

In addition to using the GENTRA Input Menu, you can enter directly in the Q1 file the GENTRA commands that define your simulation. Since the GENTRA Menu will translate your menu choices into fully commented Q1 settings, you can also edit the Q1 file to effect small modifications once the menu has taken care of the bulk of the Q1-writing work.

This chapter explains how users can avail themselves of the GENTRA-PIL for problem specification. Section 3.2 below describes the group structure of the GENTRA settings in the Q1 file; and subsequent sections deal with each GENTRA input-data group.

3.2 The Q1 file generated by the GENTRA menu

The GENTRA menu will normally be called after some provisions have been made in the Q1 file for the specification of the continuous phase (e.g., through another menu or by loading a PHOENICS Library case).

The GENTRA menu will **add** to the existing Q1 file a "GENTRA section" with the following parts:

- (a) GENTRA declarations
- (b) Groups 1 to 4: GENTRA data
- (c) Group 5: GENTRA provisions for the EARTH run
- (d) Transmission of data to EARTH

All these groups are described in the next subsections; however, you will only need to use groups 1 to 4 and (occasionally) group 5.

The Q1 file for the example of the previous chapter has been attached as Appendix E. It can be referred to for exemplification.

3.3 GENTRA declarations

The first section inserted by the GENTRA Menu into the Q1 file is used for declaration and initialisation of the GENTRA-PIL variables. Users do not need to modify in any way this section. The GENTRA PIL variables are initialised in the GENTRA Library case G0001. This is loaded by the command **L(\$G0001**, as can be seen in Group 19 of the Q1 listing in Appendix E, just before the line `GENTR = T`. It is this setting which tells EARTH that GENTRA is active.

3.4 GENTRA Groups 1 to 4: GENTRA data

This part of the Q1 file (see Appendix E for an example) carries the problem-definition settings. It comprises four groups, which are the same as those appearing in the main panel of the GENTRA menu (see figure 2.2), namely:

- | | |
|----------|-------------------------------|
| Group 1: | Particle physics. |
| Group 2: | Particle boundary-conditions. |
| Group 3: | Numerical controls. |
| Group 4: | Input/Output controls. |

Settings in these groups are effected by assigning values to the GENTRA-PIL variables. A list of these variables (and, where appropriate, the acceptable range of values) can be found in Appendix B.

GENTRA Group 2 can also carry, optionally, the inlet-data table. See Section 2.7.1 for details.

3.5 Provisions for the EARTH run

In addition to performing the data specification for the disperse phase, the GENTRA Menu will also make a number of provisions for GENTRA EARTH, such as the allocation of auxiliary storage space or the set-up of interphase sources.

The provisions made by the GENTRA Menu depend on the dimensionality of the problem, the grid type, the continuous-phase variables that are being solved for and the particle type.

The settings will be found in Groups 7, 13 and 17 of the Q1 file.

A complete list of the actions undertaken by the GENTRA Menu can be found below for the user's reference:-

- (a) If the grid is a BFC one, and the continuous-phase Cartesian velocity components UCRT, VCRT, WCRT have not been STOREd, a STORE command will be issued. (GENTRA uses the Cartesian velocity component for the integration of the particle momentum equations).

- (b) For BFC grids, NCRT (ie, the sweep frequency for the calculation of the Cartesian components in (a)) is set to 1.

- (c) 3D storage space is allocated through STORE commands for the following quantities: MOMX, MOMY, MOMZ the interphase sources of momentum. (Not stored for "lazy" and "stubborn" particles.)

HEAT, the interphase source of heat, stored if the particle is exchanging heat with the continuous phase.

MASS, the interphase source of mass, stored if the particle is exchanging mass with the continuous phase.

- (d) The variable VAPO (representing the vapour mass-fraction in the continuous phase for vaporising droplets) is SOLVED for if appropriate; and its PRANDTL numbers PRNDTL(VAPO) (laminar) and PRT(VAP0) (turbulent) are assigned according to the menu settings.

- (e) If the calculation of cell residence-time for a particle has been requested, 3D storage is allocated for the variable REST through a STORE command.

- (f) PATCHes and COVALs are generated for the interphase sources, as follows:

```
PATCH (GENPAT, CELL, 0, 0, 0, 0, 0, 0, 1, LSTEP)
COVAL (GENPAT, U1, , FIXFLU, GRND)
COVAL (GENPAT, V1, , FIXFLU, GRND)
COVAL (GENPAT, W1, , FIXFLU, GRND)
COVAL (GENPAT, H1, , FIXFLU, GRND)
COVAL (GENPAT, VAPO, FIXFLU, GRND)
```

- (g) For vaporising droplets, PATCHes and COVALs are generated for the interphase source of mass, as follows:

```
PATCH (GENMAS, CELL, 0, 0, 0, 0, 0, 0, 1, LSTEP)
COVAL (GENMAS, P1, , FIXFLU, GRND)
```

- (h) Linear relaxation is introduced for the interphase sources through the command RELAX (<var>, LINRLX, <value>), where <value> is assigned in the menu (see Section 2.8).
- (i) The call to the GENTRA Ground-station is activated by the command:
NAMGRD=GNTR

Note that, in the provisions (c), (f) and (h), the GENTRA Menu will take into account the dimensionality of the problem, and act accordingly.

3.6 Transmission to EARTH

The GENTRA-PIL variables are transmitted to EARTH through the PIL transfer arrays RG, LG, CG and IG for real, logical, character and integer variables respectively. The transmission takes via the command **L(GENSET)**, which loads GENTRA Library case G002.

The contents of this group do not need to be modified in any way. However, the RG, LG, CG or IG variables are being used for the transmission of the user's own data, please check this group for clashes with usage by GENTRA. The positions in the transfer arrays currently occupied by GENTRA are:

RG: RG(71) to RG(100)

IG: IG(9) to IG(20)

LG: LG(10) and LG(19) to LG(20)

CG: CG(6) to CG(10)

3.7 Exit and symmetry patches

Exit and symmetry patches created through Inlet, Outlet and GENTRA_SYMMETRY objects (see Section 2.7) are written to the EARDAT file directly, and do not appear in the Q1 file.

Inlets and outlets which do **not** act as GENTRA outlets have the additional line:

```
> OBJ,      GENTRA_EXIT,      1.000000E+00
```

as part of their definition. The absence of such a line is a signal that the inlet or outlet **does** act as a GENTRA exit.

GENTRA_SYMMETRY objects are written to the Q1 as:

```
> OBJ,      NAME,              name
> OBJ,      POSITION,           Xorigin, Yorigin, Zorigin
> OBJ,      SIZE,              Xsize,   Ysize,   Zsize
> OBJ,      CLIPART,           DEFAULT
> OBJ,      TYPE,              GENTRA_SYMMETRY
```

4 Running GENTRA Earth

4.1 Introduction

Chapters 2 and 3 explained how to prepare input data for GENTRA using the PHOENICS SATELLITE. This chapter explains how to run GENTRA-EARTH, and where the results of the run can be found.

4.2 The GENTRA run

GENTRA is linked in to the standard EARTH executable. To run EARTH from the VR-Environment, click on **Run, Solver**, then **Local solver (Earth)**.

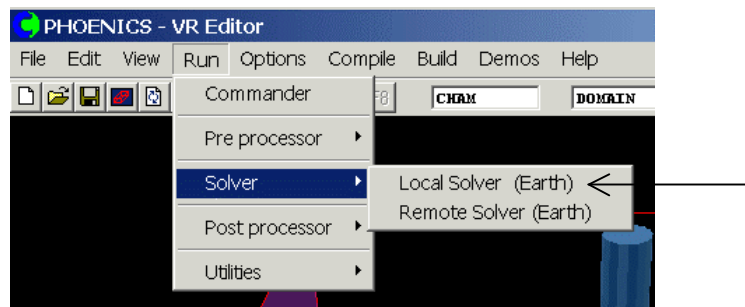


Figure 4.1: Running the EARTH Solver

The usual PHOENICS banner with the CHAM logo will be shown on the screen. If GENTRA is to be called during the run, the GENTRA banner will also be shown. The GENTRA banner contains the version number for your installation of GENTRA.

GENTRA is called at the beginning of EARTH sweeps. The first call will take place at the user-selected first GENTRA sweep, and subsequent calls will take place according to the user-selected GENTRA sweep frequency.

In each sweep, GENTRA will track the particles sequentially. Each track is started at its injection position (or at the particle position at the end of the previous time-step, if transient) and tracked until an end-of-track condition is reached. End-of-track events are:-

- (a) The particle has left the domain;
- (b) The particle has hit an obstacle and has been withdrawn;
- (c) The particle has vaporised completely;
- (d) The particle has been trapped in a stagnation region;
- (e) The tracking of the particle has timed out;
- (f) The particle was killed by the user;
- (g) The end of the Eulerian time-step (in a transient problem) has been reached;
- (h) The tracking of the particle was aborted by GENTRA.

4.3 Results produced by GENTRA

The information provided by GENTRA falls into the following categories:

- (a) Progress and error information printed on the screen;
- (b) Information in the RESULT file; and
- (c) Information in special data files.

These three categories are dealt with in the next subsections.

4.3.1 Screen information

During the GENTRA-EARTH run, a message will be written to the screen when the track for a particle starts, and another message will flag the end of the tracking and inform of the particle fate.

Between the beginning- and end-of-track flags, the following information is provided on the screen:

- Number of time-steps for the particle;
- Average number of time-steps per cell; and
- Minimum, maximum and average size of the time-step.

Error and warning messages are also routed by GENTRA to the screen.

All the output described in this section can be re-directed to a file; see Chapter 5 and Section C.3 for details.

4.3.2 The RESULT file

GENTRA itself does not print any information in the RESULT file; but the following PHOENICS quantities (provided by EARTH) are related to GENTRA calculations:

- (a) The values of MOMX, MOMY, MOMZ are the interphase sources of momentum for each cell;
- (b) the values of HEAT are the cell-values of the interphase source of heat for heat-exchanging particles;
- (c) the values of MASS are the cell values of the interphase source of mass for mass-exchanging particles; and
- (d) if the computation of particle cell-residence times is requested by the user, these will be found for each cell under the variable REST.

4.3.3 Special data files

Two special sets of files can be generated by GENTRA: one for the particle trajectories and another for particle histories (see Section 2.9 for details).

- The **trajectory** file is provided for the plotting of particle trajectories with the PHOTON post-processor. The file is read as a PHOTON geometry file, by using the command GEOMETRY READ. A trajectory file is produced for each particle. EARTH also creates a VR-Viewer macro file (PHOTON 'USE' file) called GENUSE, which draws all the saved trajectories.

A plot of the particle trajectories for the worked example of Chapter 2, created by using the GENUSE macro, can be seen in Figure 4.2.

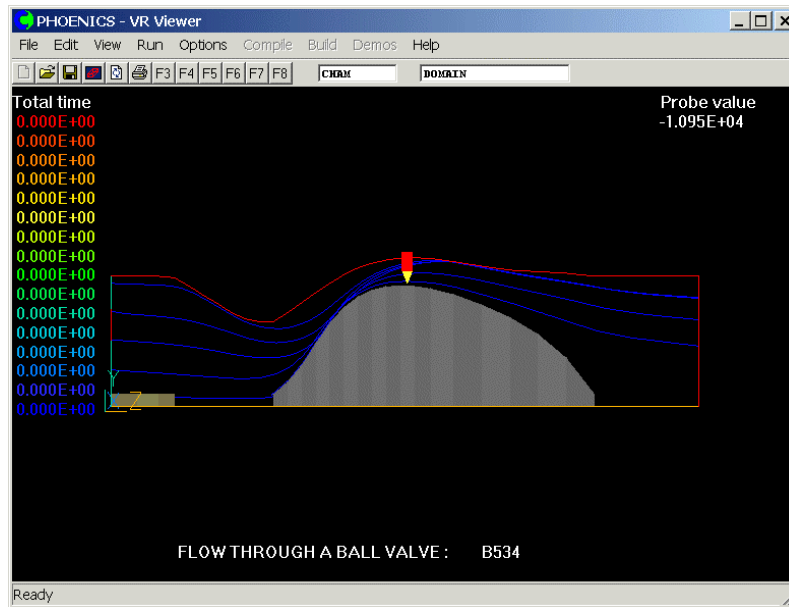


Figure 4.2: Particle tracks from the worked example

- The **history** file contains a record, in tabular format, of the evolution of the particle properties (position, velocity, temperature, size, etc) with time. This can be used by the PHOENICS post-processor Autoplot for the plotting of graphs of the x-versus-y kind. It can also, of course, be used for the user's own analysis programs.

An additional global history file may also be created. This file contains data for several particles, which can subsequently be processed to produce individual history and trajectory files. The post-processing is performed using the program UNPACK, which is executed by the command runupk. An example of the use of UNPACK is provided in Appendix K. This is not needed very often, as the Viewer can read the global history file directly.

Users with special output needs can easily create their own output by inserting the appropriate FORTRAN coding in GENIUS. Chapter 5 provides further information.

5 The GENTRA FORTRAN

5.1 Introduction

GENTRA, like PHOENICS EARTH, has a user accessible area where users can attach their own coding sequences to supplement the built-in-features. This chapter introduces this area.

5.2 The structure of GENTRA-EARTH

The EARTH part of GENTRA is attached to PHOENICS-EARTH as a `GROUND` subroutine. While most of the GENTRA-EARTH routines are supplied in binary (and are not, therefore, accessible to users) some routines are provided in open source (see figure 5.1). These are:

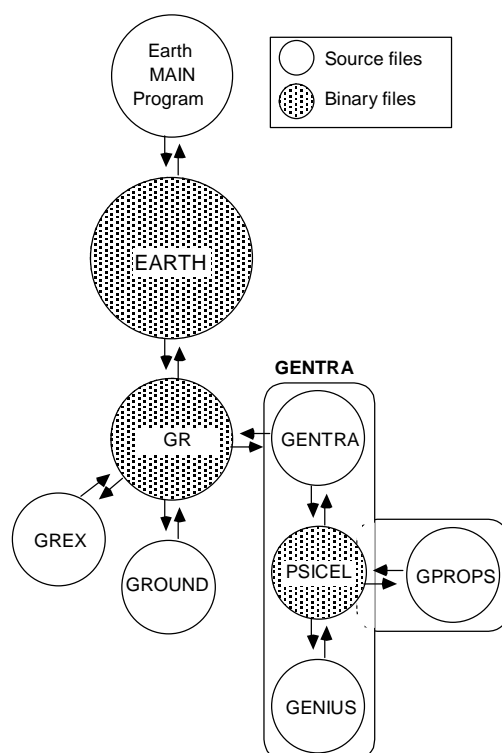


Figure 5.1: The GENTRA-EARTH structure

- **GENTRA**, the Ground Station that attaches GENTRA to EARTH. The `GENTRA` subroutine initialises the `GENTRA` variables, calls the particle-tracking modules and then transfers the interphase sources computed by `GENTRA` to the finite-volume equations solved by PHOENICS. Users seldom need to introduce changes in this module, which for this reason, is not discussed in this Guide.
- **GENIUS (GENTRA Interface for User Sequences)** is the GENTRA open-source subroutine where users can insert FORTRAN coding to supplement or replace the built-in features. `GENIUS` is called by `GENTRA` at well-defined stages during the solution of the particulate phase. `GENIUS` can therefore be regarded as the counterpart for `GENTRA` of the `EARTH GROUND`.
- **GPROPS** is the particle property function routine, in which properties of the particulate phase may be set.

Regarding the filing arrangements, all of the open-source routines are provided within the file "gentra.htm". This can be edited from the VR-Environment by clicking on **File, Open file for Editing**, and selecting **gentra**.

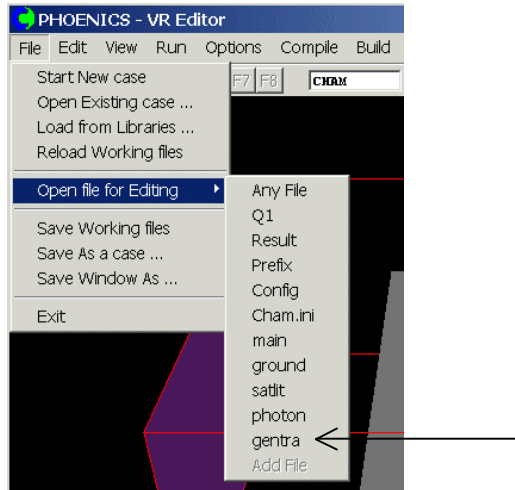


Figure 5.2: Opening GENTRA.HTM for Editing

A reference copy of this file is kept in the `\phoenics\ld_earth\ld_opt\gentra` directory. Users can copy this to their private directory for modification.

5.3 The FORTRAN subroutine GENIUS

GENIUS is similar, in concept and format, to the EARTH subroutine GROUND. GENIUS is divided into groups, some of which are further divided into sections, that are visited at specific stages during the computation. Users can insert their own coding in these groups in order to obtain additional results, to compute auxiliary data, and to influence the GENTRA computation. (Users are however advised that the modification of GENTRA variables, particularly of those which affect the particle history, should always be effected with great caution).

After a call to GENIUS, the execution is directed to the appropriate group and section by the FORTRAN variables **IGENGR (GENIUS group)** and **IGENSC (GENIUS section)** and a network of computed GOTOS. Both IGENGR and IGENSC are set within GENTRA and the user should not modify their values.

The groups and sections of GENIUS are discussed now in this guide; a list of the user-accessible FORTRAN variables can be found in Appendix C; and Appendix G contains the full listing of GENIUS.

5.3.1 GENIUS Group 1: Preliminaries

Group 1 is visited at the beginning of the first call to GENTRA in each EARTH run, ie when

```
( ISTEP.EQ.FSTEP ).AND. ( ISWEEP.EQ.GSWEP1 )
```

Group 1 is therefore a convenient place for the initialisation of local variables that are subsequently going to be used in GENIUS; and, since the group is visited after GENTRA has initialised its variables, it is also the place to override the Q1 and default settings for the GENTRA variables. Users can, for instance, change the logical units for the output files (see variables LUPRO, LUWAR, LUERR, LUTRA, LUHIS in Appendix C)

5.3.2 GENIUS Group 2: Start of new track

This group is visited at the beginning of the tracking of each particle, once:

- the particle data has been read from the inlet-data table and stored in the F-array;
- all the variables for the track (such as the particle number `IPARTI`, the absolute time `TIME`, the cell residence time `CTIME`) have been initialised; and
- the trajectory and history files have been opened (if the user has requested such output and the current sweep is the last one).

GENTRA calls this group **before** it locates, using the particle-inlet co-ordinates, the indices of the cell where the particle is initially located. Users can therefore override, in this group, the settings in the inlet-data table for the particle inlet position and properties. This is particularly useful when the particles obey a size, velocity or density distribution. In this case, “dummy” properties can be used in the inlet data, and these can be subsequently overwritten in GENIUS. To do this, the particle variables to be set in GENIUS are the ones ending in N in the list provided in Section C.2. The values will be subsequently transferred to the corresponding 0 variables by GENTRA. You do not need to supply the cell indexes `I*PAR*`, since these will be found by GENTRA using the particle co-ordinates supplied.

5.3.3 GENIUS Group 3: start of new Lagrangian time-step for the current track

Group 3 of GENIUS is visited at the beginning of the time-step, after

- the time-step counter `JCOUNT` has been updated;
- the particle properties at the beginning of the current time-step are assigned the values prevailing at the end of the previous one;
- the continuous-phase properties at the particle position have been found (see Section C.1 for a list of these variables, and Section 6.8.3 for further information); and
- the stagnation check has been passed (see Section 6.8.1);

and before

- the time-step is calculated (see Section 6.7.1); and
- the particle is moved (see Section 6.8).

Users can, in this group, specify the maximum time-step by resetting the variable `GDTMAX` (initially set in the Q1 file/menu); or inspect (and, with caution, change) the continuous-phase properties “experienced” by the particle (see Section 6.8.3).

5.3.4 GENIUS Group 4: Particle reaches cell boundary

GENIUS Group 4 is visited when a particle reaches a cell boundary. The value of `IGENSC` is used to distinguish between several events, as follows:-

<code>IGENSC=1</code>	means that the particle has reached an exit (i.e., the appropriate face of a patch whose name starts with GX);
<code>IGENSC=2</code>	means that the particle has reached a wall or obstacle. (Note that the visit to GENIUS takes place after the velocity components have been changed after bouncing, if the particle is to be bounced);
<code>IGENSC=3</code>	means that the particle has been reflected at an axis/surface of symmetry;

IGENSC=4 means that the particle is in a new cell (note that the particle might, in this case, be **inside** the new cell, and not just on the boundary).

5.3.5 GENIUS Group 5: End of current Lagrangian time-step

Group 5 of GENIUS is called at the end of the current Lagrangian time-step, after:

- the cell residence time `CTIME` and the absolute time `TIME` have been increased by `GDT`, the current time-step size;
- the several end-of-tracking criteria (such as timeouts) have been checked;
- the cell residence-time `CTIME` has been reset if the particle is in a new cell, and transferred to the full-field store in EARTH if the current particle `IPARTI` is `GRESTI`.

Users can, in group 5 of GENIUS, "kill" the tracking of the particle by setting the logical variable `KILPAR` to `.TRUE..` The tracking of the particle will be then abandoned, and GENTRA will start tracking the next one.

5.3.6 GENIUS Group 6: End of current track

Group 6 of GENIUS is visited before finishing the track for the current particle, and moving on to the next one. It is visited after the plot trajectory and history files have been written, if appropriate, and closed.

5.3.7 GENIUS Group 7: GENTRA returns control to EARTH

GENIUS Group 7 is visited immediately before RETURNING the control to EARTH, after the CALL to GENTRA for the current sweep.

5.3.8 GENIUS Group 8: Special calls

Group 8 of GENIUS is designed to allow the user to modify the built-in Lagrangian equations. There are 5 sections in this group.

- *Section 1: Particle momentum equation*

The method of discretization of the particle momentum equation is described in Section 6.5.3. The discretized form of the equations is:

$$\frac{d}{dt} \begin{bmatrix} U_p \\ V_p \\ W_p \end{bmatrix} = \text{GVCSBB}^* \begin{bmatrix} U_g \\ V_g \\ W_g \end{bmatrix} - \text{GVCSAA}^* \begin{bmatrix} U_p \\ V_p \\ W_p \end{bmatrix} + \begin{bmatrix} \text{GVCSCX} \\ \text{GVCSCY} \\ \text{GVCSCZ} \end{bmatrix}$$

At the time this section is called, all of the coefficients and sources (GVCSAA, GVCSBB, GVCSCX, GVCSCY, GVCSCZ) have been calculated in GENTRA. For the particle momentum equation given by equation (6.32) in Section 6.5.3, the prevailing values are:

$$\text{GVCSAA} = \text{GVCSBB} = D_p/m_p$$

$$\text{GVCSCX} = b \cdot g_x - \frac{1}{r_p} \cdot dp/dx$$

$$\text{GVCSCY} = b \cdot g_y - \frac{1}{r_p} \cdot dp/dy$$

$$\text{GVCSCZ} = b \cdot g_z - \frac{1}{r_p} \cdot dp/dz$$

Users are free to reset them or add to them. For example, if an extra magnetic field needs to be taken into account and the effect of the magnetic force on the particle can be written as:

$$\frac{dU_p}{dx} = \text{GMX}$$

(if only x-component of the force exists) then the user should add the following coding in this section:

$$\text{GVCSCX} = \text{GVCSCX} + \text{GMX}$$

As another example, the following coding replicates the built-in particle momentum equation:

```
REYNOL=RENLF(DIPARO,RELVEC,GSENU)
CDRG=GPROPS(1, REYNOL, GDRAG)
GVCSCX=(3.0*GSENU*DENGAS*CDRG*REYNOL)/4.0*ROPARN*DIPARO**2
GVCSCY=GVCSCX
```

where GPROPS and RENLF are GENTRA function subroutines, and all the FORTRAN variables appearing on the right hand side are in local common blocks (see the common-block file TRACMN). The values of GVCSCX, GVCSCY and GVCSCZ will already have been set in GENTRA.

- *Section 2: Particle energy equation.*

This section is called before the energy equation is solved but after the coefficients and sources (GHCSAA, GHCSBB, GHCSCC) have been calculated. The user can change the terms in the energy equation in the same way as for the momentum equation.

- *Section 3: Particle mass equation.*

This section is called before the mass equation is solved but after the coefficient and sources (GMCSAA, GMCSCC) have been calculated. Beware that instead of solving particle mass or particle diameter, the square of the particle diameter is chosen as the dependent variable.

- *Section 4: Particle solidification.*

In this section, the user can change the built-in model for particle solidification which is a function of particle temperature.

- *Section 5: User's own Lagrangian equations.*

The user can write his own particle momentum, energy, mass and solidification equations in this section. The particle velocity, temperature, size, etc., calculated here will overwrite the corresponding particle property.

5.3.9 GENIUS Group 9: Particle inlet conditions.

Whenever a data element in the particle inlet-data table described in Section 2.7.1 is replaced by the name of the data item, GENTRA will look up the relevant section in this group for the inlet data. The inlet data is passed from this section through the variable "PRVLIN". For example, if the inlet-data table reads:

```
<GENTRA-INLET-DATA>
*_ XP _ YP _ UP _ VP _ DIAM _ FRATE
  0.1 0.2 UP 1.0 1.2E-05 1.2E-03
<END-GENTRA-INLET>
```

GENIUS Group 9, Section A will be visited for the setting of UP. If the user inserts the following coding in Section 4 of this group.

```
PRVLIN=3.0
```

then the x-component of the particle velocity will be set to 3.0 m/s.

5.4 The property function - GPROPS

GPROPS is a function routine for particle properties, a full listing of which can be found in Appendix G. The arguments of GPROPS are FUNAME, PARAMT and DEFVAL. FUNAME is the index number of the function (eg 4 for the thermal conductivity of the vapour), PARAMT is the main parameter of which GPROPS is a function, and DEFVAL is the default value for the function. If DEFVAL is not a GROUND number, GPROPS is set to DEFVAL before returning. However, if DEFVAL is equal to a GROUND number, control will be directed within GPROPS to the appropriate section where it will be set as a function of PARAMT. It is possible to set GPROPS to be a function of any of the variables within GENTRA (described in Appendix C), as these are available within GPROPS due to the inclusion of the common file "TRACMN". If a GROUND number is set for DEFVAL, but appropriate coding is not supplied within GPROPS, an error condition will occur and execution of GENTRA-EARTH will be stopped.

5.5 Building private versions of GENTRA

After modifying a user-accessible module of GENTRA (i.e., subroutines GENTRA, GENIUS or GPROPS), the user must build a private version of EARTH. The build script will automatically compile GENTRA.HTM, so there is no real need to compile it separately.

In the VR-Environment, click on **Build**, then **Earth**.

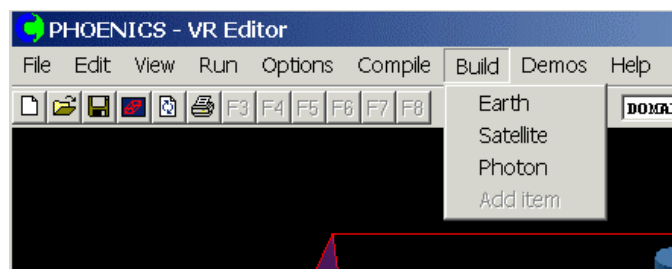


Figure 5.3: Building a 'Private' EAREXE

Once the new EARTH executable has been built, the environment must be told to run the 'private' EARTH, not the 'public' (CHAM-supplied) EARTH. Click on **Options**, **Run version**, then select '**Private**' or '**Prompt**' for Earth.

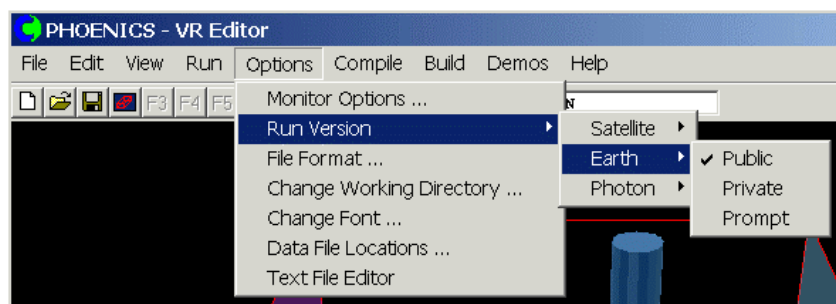
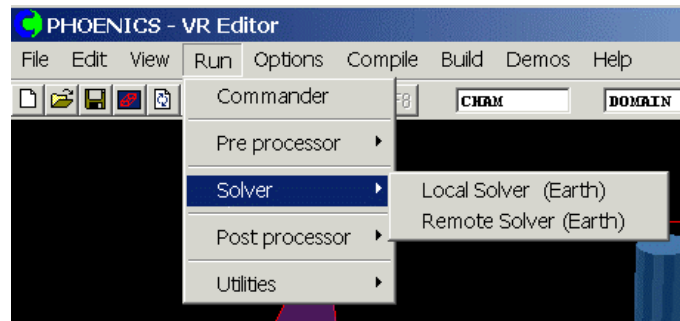


Figure 5.4: Selecting to run a 'Private' EAREXE

To run EARTH, click on Run, Solver, Local Solver (Earth). If 'private' had been selected above, the newly-built EARTH executable will be run. If '**Prompt**' had been selected, the option of running 'Private' or 'Public' EARTH will be offered.

**Figure 5.5: Running the EARTH Solver**

6 The GENTRA Equations

6.1 Introduction

As pointed out in Chapter 1, GENTRA uses Lagrangian equations for the representation of the particulate phase. These equations are listed in the present chapter, in which some details of the integration procedure are also given.

It should be pointed out that users do not need to be acquainted with the contents of this chapter to be able to operate GENTRA successfully; the chapter is therefore provided as a reference for users who need to be concerned with the mathematical basis of GENTRA.

6.2 The continuous-phase equations

GENTRA uses, for the description of the continuous phase, the Eulerian equations built in PHOENICS for single-phase flows, which have the general form:

$$\frac{\partial}{\partial t}(r_c f_c) + \nabla \cdot (\mathbf{U}_c \rho_c \phi_c) - \nabla \cdot (\Gamma \nabla \phi_c) = S_\phi + S_{\phi G} \quad [6.1]$$

where

- ϕ_c is the continuous-phase property modelled;
- ρ_c is the continuous-phase density;
- \mathbf{U}_c is the continuous-phase velocity;
- Γ is an exchange coefficient for ϕ_c ;
- S_ϕ are the sources/sinks of ϕ_c ; and
- $S_{\phi G}$ are the interphase sources computed by GENTRA and accounting for the transfer of ϕ_c between the phases.

Equations such as equation (6.1) are set up by PHOENICS following the instructions supplied by the user through the PHOENICS Input Language or a PHOENICS menu.

The variables ϕ_c for which GENTRA will expect PHOENICS to solve equations like equation (6.1) vary from problem to problem, as follows:

- (a) For all particle types, except for stubborn particles, GENTRA requires the velocity component in each of the co-ordinate directions considered (U1/V1/W1)
- (b) For particles with heat transfer, melting/solidifying particles and vaporising droplets, an equation for enthalpy H1, or temperature, TEM1, is also required.
- (c) For vaporising droplets, the mass-transfer term ($S_{\phi G}$ in equation 6.1) is inserted into the equation for P1 (which in PHOENICS is the continuity/pressure correction equation); and a transport equation must also be set up for VAPO, the mass fraction of droplet vapour in the continuous phase.
- (d) When the stochastic turbulence model is used, the equations for KE (turbulence kinetic energy) and EP (its rate of dissipation) must also be solved.

The solution of the above variables can be replaced by the simple storage (without solution) of their values when GENTRA is to track the particles through a "frozen" flow-field.

6.3 Lagrangian equations

In the simulation of particle behaviour, Lagrangian equations are solved which describe the evolution of the position, velocity (momentum), mass and temperature (enthalpy) of the particle. Some combination of these equations is employed for the different types of particle available within GENTRA as detailed in Section 2.5. In the following sub-sections, descriptions are presented of each of the Lagrangian equations, and their relevance to each of the particle types is discussed. The method of integration of these equations is explained in Section 6.5.

6.3.1 The particle position equation

The evolution of the particle position is determined from solution of the following equation:

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{U}_p \quad [6.2]$$

where vector \mathbf{x}_p is the particle position; and \mathbf{U}_p is the particle velocity. Generally, the particle velocity is determined from solution of the particle momentum equation, as described in Section 6.3.2. However, for lazy and stubborn particles, the particle velocity is calculated as follows:

- **Lazy particles.** For lazy particles it is assumed that the particle velocity is identical to the instantaneous continuous-phase velocity:

$$\mathbf{U}_p = \mathbf{U}_c + \mathbf{U}_c'$$

where: \mathbf{U}_c is the time-averaged continuous-phase velocity; and \mathbf{U}_c' is a turbulent velocity fluctuation calculated from the local turbulence conditions when the stochastic turbulence model is activated.

- **Stubborn particles.** For stubborn particles, the particle velocity is constant and equal to the value prescribed at the inlet.

$$\mathbf{U}_p = \text{constant}$$

6.3.2 The particle momentum equation

The velocity of the particle, \mathbf{U}_p , is computed from the particle momentum equation:

$$m_p \frac{d\mathbf{U}_p}{dt} = D_p(\mathbf{U} - \mathbf{U}_p) + m_p b \mathbf{g} - V_p \tilde{N}_p \quad [6.3]$$

where

m_p is the mass of the particle;

D_p is a drag function, to be defined below;

\mathbf{U} is the continuous-phase instantaneous velocity, $\mathbf{U} = \mathbf{U}_c + \mathbf{U}_c'$. \mathbf{U}_c is the continuous-phase average velocity, and \mathbf{U}_c' is a turbulent fluctuation which is added if the stochastic turbulence-model is active (see Section 6.4.1);

g is the gravitational acceleration;

b is a buoyancy factor, equal to $(1 - \frac{\rho_c}{\rho_p})$ if the buoyancy option is active or to 1.0 otherwise;

V_p is the particle volume; and

\tilde{N}_p is the continuous-phase pressure gradient.

The first term on the right-hand side of equation (6.3) represents the drag force exerted by the continuous phase on the particle; and the second represents the gravitational force. Source terms accounting for the virtual mass and Basset forces, Saffman lift and Magnus forces are neglected. The conditions under which these source terms can be neglected have been given by Faeth (1983).

The drag function D_p used in GENTRA has the following form:

$$D_p = \frac{1}{2} \rho A_p C_D |\mathbf{U} - \mathbf{U}_p| \quad [6.4]$$

where

$$A_p \text{ is the particle projected area, } \frac{\pi d_p^2}{4} \quad [6.5]$$

C_D is the drag coefficient, which by default is given by

$$C_D = \frac{24}{Re} (1 + 0.15 Re^{0.687}) + \frac{0.42}{1 + 4.25 \cdot 10^4 Re^{-1.16}} \quad [6.6]$$

where Re is the particle Reynolds number.

(This correlation, provided by Clift, Grace and Weber (1978), is valid for rigid spherical particles and $Re < 3 \times 10^5$)

6.3.3 The particle mass equation

The evolution of the mass of the particle, m_p , is described by the particle mass equation, thus:

$$\frac{dm_p}{dt} = - \pi d_p \frac{k_v}{c_{pv}} Nu \ln(1 + B_M) \quad [6.7]$$

where:

d_p is the diameter of the particle;

k_v is the thermal conductivity of the vapour produced by the evaporation of the droplet;

c_{pv} is the specific heat capacity of that vapour;

Nu is the Nusselt number, determined from the following correlation:

$$Nu = 2(1 + 0.3 Re^{0.5} Pr^{0.33}) F \quad [6.8]$$

where: Pr is the laminar Prandtl number for the continuous phase; and
 F is the Frossling correction for mass transfer, given by:

$$F = \frac{1}{B_M} \ln (1 + B_M) \quad [6.9]$$

B_M is the mass transfer number, which represents the "driving force" in the mass transfer process, and is defined by:

$$B_M = \left[\frac{Y_{vs} - Y_{v\infty}}{1 - Y_{vs}} \right] \quad [6.10]$$

where:

Y_{vs} is the mass fraction of vapour at the surface of the droplet; and

$Y_{v\infty}$ is the mass fraction of vapour in the gas surrounding the droplet.

The mass fraction of vapour at the surface of the droplet is calculated thus:

$$Y_{vs} = \left[1 + \left(\frac{P}{P_{vs}} - 1 \right) \frac{W_c}{W_v} \right]^{-1} \quad [6.11]$$

where:

P is the total pressure of the fluid surrounding the droplet;

P_{vs} is the partial pressure of the vapour at the surface of the droplet at the saturation conditions defined by the droplet temperature;

W_c is the molecular weight of the surrounding fluid; and

W_v is the molecular weight of the vapour.

Within GENTRA, the mass transfer equation is employed only in the simulation of vaporising droplets.

6.3.4 The particle enthalpy equation

The temperature of the particle, T_p , is determined from solution of the particle enthalpy equation. In its most general form, the particle enthalpy equation may be written:

$$m_p C_p \frac{dT_p}{dt} = m_p L \frac{df_s}{dt} + H_{fg} \frac{dm_p}{dt} + \alpha (T_g - T_p) \quad [6.12]$$

where:

C_p is the specific heat capacity of the particle;

L is the latent heat of solidification;

H_{fg} is the latent heat of evaporation;

f_s is the proportion of the solid phase in the particle (the solid fraction);

α is the heat transfer coefficient between the particle and the surrounding fluid; and

T_g is the temperature of the surrounding fluid.

The specific heat capacity of the particle may be a function of both the temperature and the composition of the particle, thus:

$$C_p = f_s (C_{ps} (T_p)) + (1 - f_s) (C_{pl} (T_p)) \quad [6.13]$$

where C_{ps} and C_{pl} represent the specific heats of the solid and liquid phases of the particle as functions of the particle temperature.

The latent heat of solidification of the particle is defined as the difference in total enthalpy of the solid and liquid phases at a given temperature:

$$L = h_{l0} + \int_0^T C_{pl} dT - (h_{s0} - \int_0^T C_{ps} dT) \quad [6.14]$$

where:

h_{s0} is the enthalpy of the solid phase at the reference temperature of 0.0 K; and

h_{l0} is the enthalpy of the liquid phase at the same reference temperature.

In the case of the specific heat capacities of the two phases being equal, the latent heat of solidification is independent of temperature and equal to $h_{l0} - h_{s0}$.

The solid fraction of the particle is determined from the following equation:

$$f_s = \left[\frac{T_L - T_p}{T_L - T_S} \right]^m \quad [6.15]$$

where:

T_S is the solidus temperature of the particle;

T_L is the liquidus temperature of the particle; and

m is the solidification index.

The particle heat transfer coefficient, α , is determined from:

$$\alpha = \pi k_c Nu d_p \quad [6.16]$$

where k_c is the thermal conductivity of the continuous phase.

The particle enthalpy equation is not used in the simulation of lazy, stubborn or isothermal particles. For the other particle types, it is employed in the following reduced forms:

Heat exchanging particles:

$$m_p C_p \frac{dT_p}{dt} = \alpha (T_g - T_p) \quad [6.17]$$

in which the terms representing solidification/melting and evaporation are absent.

Melting/solidifying particles:

$$m_p C_p \frac{dT_p}{dt} = m_p L \frac{df_s}{dt} + \alpha (T_g - T_p) \quad [6.18]$$

in which the term representing evaporation is not present.

Vaporising droplets:

$$m_p C_p \frac{dT_p}{dt} = H_{fg} \frac{dm_p}{dt} + \alpha (T_g - T_p) \quad [6.19]$$

in which the solidification term is absent.

6.4 Submodels**6.4.1 Stochastic turbulence model**

GENTRA features an optional stochastic turbulence model (Gosman and Ioannides, 1981) which accounts for the effects on particle dispersion of the turbulent fluctuations of the continuous-phase velocity.

The model uses, as the continuous-phase velocity in the drag force term of the momentum equation (equation (6.3)), a sum of the average velocity \mathbf{U}_c and a "fluctuating" component \mathbf{U}'_c :

$$\mathbf{U} = \mathbf{U}_c + \mathbf{U}'_c \quad [6.20]$$

where:

\mathbf{U}_c , the average velocity, is obtained from the Eulerian equations for the continuous phase; and

\mathbf{U}'_c , the fluctuating component, is calculated assuming that each component follows a normal distribution with a mean value of 0.0 and a standard deviation of

$$\sigma = \sqrt{2K/3} \quad [6.21]$$

where K is the turbulence kinetic-energy.

The fluctuating component \mathbf{U}'_c is assumed to act over a time interval Δt_s which is the minimum of:-

- (a) Δt_e , the lifetime of the local eddy which the particle is assumed to be traversing; and
- (b) Δt_r , the transit time taken for the particle to cross the eddy.

The eddy lifetime Δt_e is computed as:

$$\Delta t_e = \frac{l_e}{|\mathbf{U}'_c|} \quad [6.22]$$

where l_e is the eddy size:

$$l_e = \frac{C_\mu^{3/4} K^{3/2}}{\varepsilon} \quad [6.23]$$

where: ε is the rate of dissipation of turbulence kinetic energy, and C_μ is a constant in the turbulence model.

The particle transit-time Δt_r is given by

$$\Delta t_r = \frac{l_e}{|\mathbf{U} - \mathbf{U}_p|} \quad [6.24]$$

6.4.2 Rotating-coordinate systems

In rotating-coordinate systems, the particle (\mathbf{U}_p) and continuous-phase (\mathbf{U}_c) velocities solved for by GENTRA and PHOENICS are the ones **relative** to the rotating system. Coriolis and centrifugal sources must therefore be included in the momentum equations.

For the particle, the extra term in the momentum equation (equation (6.3)) is:

$$\mathbf{S}_p = -m_p [2.\boldsymbol{\Omega} \times \mathbf{U}_p + \boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \mathbf{x}_p)] \quad [6.25]$$

where:

$\boldsymbol{\Omega}$ is the angular speed of rotation (expressed here as a vector along the axis of rotation);

\mathbf{x}_p is the particle-position vector; and

\times indicates cross product.

The rotating-co-ordinate feature of GENTRA is activated automatically when its PHOENICS counterpart is activated. See the entry ROTA in the SATELLITE help dictionary for details on how to activate it and how to specify the axis of rotation and the angular speed.

(Note that the FORTRAN logical variable ROTCOO can be used to **deactivate** the automatic introduction of this feature. See Appendix C for details).

6.5 Integration of the equations

The numerical integration of the particle equations takes place according to the following sequence:-

- (a) The Lagrangian time-step is calculated;
- (b) The particle is moved;
- (c) The particle properties at the new position are calculated;
- (d) The interphase sources are calculated.

These four steps are dealt with in subsequent subsections.

6.5.1 Calculation of the Lagrangian time-step Δt_l

The Lagrangian time-step is computed by GENTRA as:-

$$\Delta t_l = \max (\tau_0, \min (\tau_1, \tau_2, \tau_3)) \quad [6.26]$$

where τ_0 to τ_3 are as follows:

(a) τ_0 is a **minimum** time-step size, given by the FORTRAN variable GDTMIN. Its default value is 10.0^{-7} ; users can re-set it in Group 1 of GENIUS.

(b) τ_1 is the minimum cell-crossing time divided by the Q1-set variable GLAGTS (the minimum number of Lagrangian time-steps per cell specified by the user). The minimum cell-

crossing time is **estimated** by GENTRA for each cell using the minimum cell dimension and the maximum velocity component.

(c) τ_2 is the momentum relaxation time.

If the particle momentum equation is re-written as

$$\frac{d\mathbf{U}_p}{dt} = A - B \mathbf{U}_p \quad [6.27]$$

τ_2 is calculated as $\frac{\alpha}{B}$, where α is a multiplication factor.

α is available (through GENIUS) as the FORTRAN variable GRTFRL. Its default value of 10^{10} effectively excludes τ_2 as a criterion in equation (6.26) (since it is larger than the others).

Users wanting to relate the time-step Δt_i to the momentum relaxation-time τ_2 can reset GRTFRC in Group 1 of GENIUS. However, this might result in very small time-steps for small particles.

(d) τ_3 is the user-supplied maximum time-step size (PIL variable GDTMAX).

Note that the time step thus computed may be further reduced by GENTRA after the integration of the position equations as follows:

- (a) The particle is not allowed to jump, in the current time-step, beyond the neighbouring cells;
- (b) for boundary cells (i.e., cells at the boundaries of the computational domain or cells next to internal blockages), a particle crossing the cell boundary is placed **on** the cell boundary by reducing the time-step.

6.5.2 Moving the particle

After computing the time-step Δt_i , the particle is "moved" by integrating the particle-position equations. The particle-position equation (equation (6.2))

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{U}_p$$

is integrated as:

$$\mathbf{x}_p^n = \mathbf{x}_p^o + \mathbf{U}_p^o \Delta t \quad [6.28]$$

where:

n denotes the value at the **end** of the time step; and

o denotes the value at the beginning of the time-step.

GENTRA integrates the position equations in the GENTRA Cartesian System; in cylindrical-polar grids, equation (6.28) can optionally be integrated in polar co-ordinates (i.e., using the radius, the angle and the circumferential and radial velocities as variables). The FORTRAN logical variable POLTRC (see Appendix C), accessible from GENIUS, controls this option. (Note, however, that, in order to avoid the singularity at the polar axis $y=0$, GENTRA will always track in Cartesian co-ordinates in the centre of the grid (IY=1).)

6.5.3 Integration of momentum, mass and enthalpy equation

The equations representing the momentum, mass and enthalpy of the particles can be represented in the following generalized form.

$$\frac{d\xi}{dt} = A - B\xi \quad [6.29]$$

where ξ represents the variable to be solved (i.e. momentum, mass or enthalpy), and A and B are constants.

The equation is integrated over the Lagrangian time step Δt_l such that the value at the end of the time step, ξ^n , can be expressed in terms of the value at the start of the time step, ξ^0 , and the constants A and B, thus:

$$\xi^n = \xi^0 e^{-B\Delta t_l} + \frac{A}{B}(1 - e^{-B\Delta t_l}) \quad [6.30]$$

If the constant, B, in equation (6.29) is zero, implying that the rate of change of ξ is independent of the value of ξ , the use of equation (6.30) would result in division by zero. Hence, in this case, equation (6.29) is integrated thus:

$$\xi^n = \xi^0 + A\Delta t \quad [6.31]$$

The form of the constants in equation (6.29) is dependent on the equation being solved. In the following subsections, the method of integration for each of the particle equations will be presented.

The particle momentum equation

The particle momentum equation (equation (6.3)), may be expressed in the form of equation (6.29) as:

$$\frac{dU_p}{dt} = \frac{D_p \mathbf{U}_g}{m_p} + b\mathbf{g} - \frac{D_p}{m_p} U_p - \frac{1}{r_p} \tilde{N}_p \quad [6.32]$$

from which the constants A and B of equation (6.29) can be seen to be:

$$A = \frac{D_p}{m_p} \mathbf{U}_g + b\mathbf{g} - \frac{1}{r_p} \tilde{N}_p \quad [6.33a]$$

$$B = \frac{D_p}{m_p} \quad [6.33b]$$

The particle mass equation

For the case of a particle evaporating in a constant environment, and at constant temperature, the rate of change of particle surface area with time is constant. This is taken into account in the method employed for the integration of the particle mass equation, which is cast into the form of an equation for the rate of change of particle surface area (d_p^2), thus:

$$\frac{d(d_p^2)}{dt} = \frac{-4}{\rho_p} \frac{k_v}{C_{pv}} \text{Nu} \ln(1+B_M) \quad [6.34]$$

This is integrable using equation (6.31), in which the constant, A, is equal to the right hand side of equation (6.34):

$$A = \frac{-4}{\rho_p} \frac{k_v}{C_{pv}} \text{Nu} \ln(1+B_M) \quad [6.35]$$

The rate of change of particle mass is then deduced from the change in particle diameter.

The particle enthalpy equation

The particle enthalpy equation its most general form is given by equation (6.12), thus:

$$m_p C_p \frac{dT_p}{dt} = m_p L \frac{df_s}{dt} + H_{fg} \frac{dm_p}{dt} + \alpha(T_g - T_p)$$

Before integrating this, the solidification/melting term is expressed in a more useful form by noting the relation between the solid fraction, f_s , and the particle temperature, T_p , equation (6.15):

$$f_s = \left[\frac{T_L - T_p}{T_L - T_S} \right]^m$$

This can be differentiated with respect to the particle temperature, yielding:

$$\frac{df_s}{dT_p} = -m \frac{(T_L - T_p)^{m-1}}{(T_L - T_S)^m} \quad [6.36]$$

and the original term representing the rate of change of solid fraction with time can be expressed as:

$$\frac{df_s}{dt} = -m \frac{(T_L - T_p)^{m-1}}{(T_L - T_S)^m} \frac{dT_p}{dt}$$

This may be substituted into the general particle enthalpy equation, which may be written in the form of the general particle equation (equation (6.29)):

$$\frac{dT_p}{dt} = \frac{\alpha T_g + H_{fg} dm_p/dt}{m_p [C_p + Lm + Q]} - \frac{\alpha T_p}{m_p [C_p + Lm + Q]} \quad [6.37]$$

where:

$$Q = \frac{(T_L - T_p)^{m-1}}{(T_L - T_S)^m} \quad [6.38]$$

This may then be integrated via equation (6.30).

For the three types of particles involving heat exchange which are available in the current version of GENTRA (ie heat exchanging, melting/solidifying and vaporizing), some terms of the general enthalpy equation are absent. For each of these particle types, there now follows the form of equation (6.37) which is employed.

Heat exchanging particles:

$$\frac{dT_p}{dt} = \frac{\alpha T_g}{m_p C_p} - \frac{\alpha T_p}{m_p C_p} \quad [6.39]$$

Melting/solidifying particles:

$$\frac{dT_p}{dt} = \frac{\alpha T_g}{m_p [C_p + Lm + Q]} - \frac{\alpha T_p}{m_p [C_p + Lm + Q]} \quad [6.40]$$

Vaporising droplets:

$$\frac{dT_p}{dt} = \frac{\alpha T_g + H_{fg} dm_p/dt}{m_p C_p} - \frac{\alpha T_p}{m_p C_p} \quad [6.41]$$

6.5.4 Calculation of sources

As the particles traverse each cell, exchange of mass, momentum and enthalpy may occur. For example, a particle which is travelling faster than the surrounding fluid will be decelerated and will transfer momentum to that fluid. The sources which must be added to the continuous-phase transport equations to represent these transfers are as follows.

Mass transfer

$$S_m = \frac{\pi}{6} \sum \eta [\rho_p^o (d_p^o)^3 - \rho_p^n (d_p^n)^3] \quad [6.42]$$

where:

n denotes values at the end of the Lagrangian time step;

o denotes values at the start of the Lagrangian time step;

η is the number flowrate of particles for that parcel (ie the mass flowrate of that parcel divided by the mass of an individual particle); and

\sum is the summation over all of the Lagrangian time steps required for the particle to traverse the cell, and for all particles.

The mass added to the continuous-phase continuity equation represents fluid evaporated from the droplet surfaces. A PHOENICS transport equation (such as equation (6.1)) is solved for the vapour mass fraction, and sources must also be added to this equation to account for the vapour added from the particles. The source in the vapour mass fraction equation is identical to that added to the continuity equation.

Momentum transfer

The source of momentum, S_{mom} , which appears in the continuous-phase momentum equations is equal to the rate of change of particle momentum as each particle parcel traverses a cell:

$$S_{mom} = \frac{\pi}{6} \sum \eta [\rho_p^o V_p^o (d_p^o)^3 - \rho_p^n V_p^n (d_p^n)^3] \quad [6.43]$$

where V_p is the particle velocity integrated from the momentum equation without body forces.

Enthalpy transfer

The source of enthalpy, S_h , which appears in the continuous-phase enthalpy or temperature equation is:

$$S_h = \frac{\pi}{6} \sum \eta [\rho_p^o h_p^o (d_p^o)^3 - \rho_p^n h_p^n (d_p^n)^3] \quad [6.44]$$

where h_p is the enthalpy of the particle relative to a value of zero at 0.0 K.

6.6 Additional information

6.6.1 Stagnation criterion

GENTRA will automatically detect whether a particle has fallen into a stagnation region, and will stop the tracking of the particle if no heat or mass-transfer effects are to be considered. The stagnation criterion is based on the continuous-phase velocity ($|\mathbf{U}_c|$), the particle velocity ($|\mathbf{U}_p|$) and a characteristic velocity (U_{char}). The tracking of the particle is abandoned if

$$\frac{|\mathbf{U}_c| + |\mathbf{U}_p|}{U_{char}} < r \quad [6.45]$$

where r is a constant.

The characteristic velocity U_{char} is computed for each time-step as the maximum of $|\mathbf{U}_c|$, $|\mathbf{U}_p|$ and the existing value of U_{char} .

The FORTRAN variables representing the different elements of equation (6.45) are as follows:

$|\mathbf{U}_c|$ is `GVFLOW`; it can be inspected by the user in `GENIUS`, but it is set **only** by `GENTRA`;

$|\mathbf{U}_p|$ is `GVPART`; it can be inspected by the user in `GENIUS`, but it is set **only** by `GENTRA`;

U_{char} is `CHARVL`; it can be set by the user in `GENIUS` (eg in Group 3), but the maximum value referred to above will nevertheless be taken by `GENTRA`, and U_{char} will be accordingly changed; and

r is `STARAT`; it has a default value of 0.01, but it can be set by the user at the beginning of the `GENTRA` run (`GENIUS` Group 1), of the track (`GENIUS` Group 2) or of the time-step (`GENIUS` Group 3).

6.6.2 Particle bouncing

When a particle tries to cross into a wall or obstacle during a time-step, `GENTRA` will reduce the time-step so that the particle is placed **on** the wall or obstacle surface. If the user has specified that the particle is to be bounced with a given restitution coefficient, the particle velocity is modified as follows (see figure 6.1):

- (a) The velocity component parallel to the wall after the bounce equals the same component **before** the bounce.
- (b) The velocity component perpendicular to the wall after the bounce is set to the negative of the same component before the bounce multiplied by the restitution coefficient.

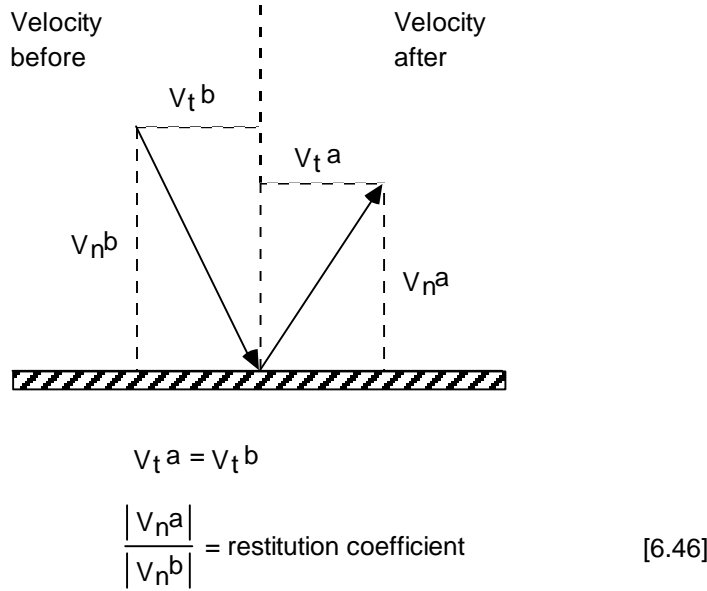


Figure 6.1: Particle bouncing

6.6.3 Fluid properties at the particle position

The fluid properties at the particle position are computed by GENTRA as follows:

- For the velocity components in Cartesian and cylindrical polar grids, the value is interpolated at the particle position using the values at the two neighbouring nodes.
- For all the other variables, and for the velocity resolute in BFC cases, the fluid properties "experienced" by the particle are those prevailing at the cell centre.

The FORTRAN variables which carry the fluid properties "experienced" by the particle are those listed in Appendix C. Users with special needs can modify the values of these variables in GENIUS Group 3 (see Section 5.3.3).

6.6.4 Particle volume fraction

For steady flows (STEADY=T), when STORE(PVFR) appears in the Q1 file, or when the particle index for the calculation of residence time is set to -2 (see Section 2.9.3), a particle volume-fraction ε_p is computed for each cell as:-

$$\varepsilon_p = \sum_{k=1}^N \frac{V_k \eta_k \Delta t_k}{V_{cell}} \quad [6.47]$$

where k represents a parcel of particles; V_k is the volume of each particle; η_k is the number flow-rate for the parcel; Δt_k is the residence time of the parcel in the cell; and V_{cell} is the cell volume.

For unsteady flows (STEADY=F), when STORE(PVFR) appears in the Q1 file (see Section 2.9.3), a particle volume fraction is computed for each cell as:

$$\varepsilon_p = \sum_{k=1}^N \frac{V_k}{V_{cell}} \quad [6.48]$$

6.6.5 Particle mass concentration

When STORE(PMCO) appears in the Q1 file (see Section 2.9.4), a particle mass concentration C_p is computed for each cell.

For steady flows, the particle mass concentration is computed for each cell as:

$$C_p = \sum_{k=1}^N \frac{\rho_k V_k h_k \Delta t_k}{V_{cell}} \quad [6.49]$$

where ρ_k is the density of each particle. For unsteady flows, it is computed for each cell as:-

$$C_p = \sum_{k=1}^N \frac{\rho_k V_k}{V_{cell}} \quad [6.50]$$

6.6.6 Mixture density

When STORE(RHMX) appears in the Q1 file (see Section 2.9.5), a mixture density is computed for each cell as:-

$$\rho_m = \rho_c (1 - e_p) + C_p \quad [6.51]$$

where ρ_c is the density of the continuous phase, .

6.6.7 Particle mass fraction

When STORE(PMFR) appears in the Q1 file (see Section 2.9.6), a particle mass fraction Y_p is computed for each cell as:-

$$Y_p = \frac{C_p}{\rho_m} \quad [6.52]$$

Appendix A. Known Limitations of GENTRA

This entry provides a summary of those limitations of GENTRA known to the GENTRA Development Team at CHAM. The list is not intended to be exhaustive; but the main limitations are nevertheless listed and, where possible, alternatives are suggested.

Most of these limitations will be removed in future versions of the software.

BFC GRIDS

Only right-handed XYZ and IJK systems are allowed.

Two-dimensional BFC grids are treated internally as having a uniform thickness in the third direction equal to XULAST, YVLAST or ZWLAST as appropriate. (Note that this is an INTERNAL arrangement that does not affect the user, other than that trajectories will only appear correct if viewed head-on with no perspective.)

CHEMKIN

GENTRA cannot be used in combination with the PHOENICS-CHEMKIN interface without user intervention. The reason is that GENTRA operates in SI units, whereas CHEMKIN employs cgs units.

CYCLIC BOUNDARY CONDITIONS

In BFC cases, only cyclic boundaries which are coincident in physical space may be used.

FIXVAL OBSTACLES

GENTRA will not recognise obstacles that are represented by FIXVALing the velocity components to zero, as is the case at the surface of solids in conjugate heat-transfer problems. However, in such problems a property index field (PRPS) is stored, the value of which denotes the material or fluid in each cell. PRPS values greater than a certain number (99 by default) represent solid materials and GENTRA tests the PRPS field if it is stored to determine the presence of solid obstructions.

This method cannot be applied to locate cell faces which have been blocked by fixing the velocities to zero (and which would therefore represent thin plates).

However, users can represent these obstacles by, in addition to FIXVALing the velocities to 0, using a porosity of 0.999 and alter accordingly the porosity threshold of GENTRA in the BOUNDARY CONDITIONS section. A porosity of 0.999 will then be recognised by GENTRA as an obstacle, while leaving the domain virtually unblocked for the diffusion of the continuous phase.

Fine-Grid Embedding

GENTRA is not compatible with the use Fine-Grid Volume objects.

GCV and CCM

GENTRA is not compatible with the GCV or CCM forms of BFC, in single or multi-block form.

OUT-OF-CORE MODE

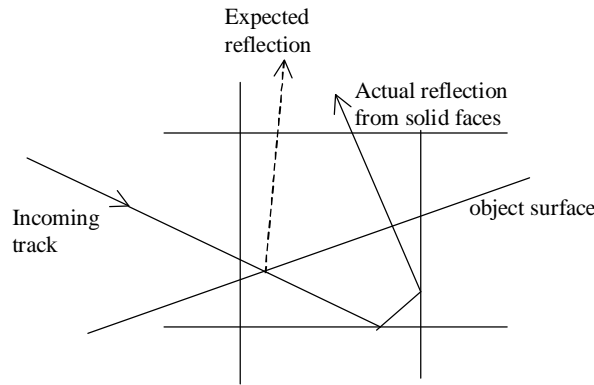
The out-of-core device of PHOENICS cannot be used with GENTRA.

PARABOLIC MODE

GENTRA does not work with the parabolic solution-procedure of PHOENICS (PARAB=T).

PARSOL

If GENTRA is used in conjunction with PARSOL (Partial Solids treatment), inaccurate trajectories near object surfaces may result. This is because GENTRA treats all partially-blocked cells as completely fluid, and will bounce particles from the faces of the first fully-blocked cell, not the true surface of the object.



PARTICLE-TO-PARTICLE INTERACTIONS

Particle-to-particle effects (such as particle collision and droplet coalescence) are not considered.

RINNER

In cylindrical-polar grids, the PHOENICS variable RINNER (which specifies the inner radius of the computational domain) must be 0 if GENTRA is used.

Annular geometries may be represented by specifying RINNER=0.0, and setting the dimension of the first radial cell (IY=1) to be the required inner radius of the annulus.

The cells at IY=1 should then be blocked with porosities (i.e. CONPOR(0.0,CELL,1,NX,1,1,1,NZ)).

TURBULENCE MODULATION

Turbulence modulation (the effect of the presence of particles on the continuous-phase turbulence) is not considered.

TWO-PHASE FLOWS

GENTRA has not yet been used in conjunction with the Eulerian-Eulerian two-phase capabilities of PHOENICS (ONEPHS=F). However, there is no built-in limitation in this respect. (Note that, if used in two-phase mode, phase-1 variables would be used as representing the continuous-phase flow-field.)

VOLUME-DISPLACEMENT EFFECTS

Volume-displacement effects (ie, the volume occupied by the disperse phase and therefore unavailable to the continuous phase) are not considered in GENTRA.

WALLS

GENTRA will automatically detect internal and boundary walls; however, all moving walls will be interpreted as being stationary for the particles.

Appendix B. List of GENTRA PIL variables

B.1 Introduction

This chapter lists all the GENTRA-PIL variables, with their type, default value and, if appropriate, units and valid range of values (the latter enclosed in angle brackets <>). See Chapter 3 for background information on the GENTRA-PIL.

In addition to being used in the Q1 file, all these variables are also available in the FORTRAN subroutine GENIUS through the COMMON blocks INCLUDED in TRACMN.

Information on each of these variables is also available through the GENTRA Menu. See Section 2.5.

B.2 List of variables

B.2.1 GENTRA Group 1: Particle physics

Variable	Type	Meaning
GBUOYA	BOOL	Switch for buoyancy effect
GCPCON	REAL	Cp of continuous phase
GCPLIQ	REAL	Cp of particle or Cp of liquid for solid/melt particle
GCP SOL	REAL	Cp of solid
GCPVAP	REAL	Cp of Vapour
GDRAG	REAL	Drag coefficient
GGRAX	REAL	X-component of gravity vector
GGRAY	REAL	Y-component of gravity vector
GGRAZ	REAL	Z-component of gravity vector
GHLIQD	REAL	Particle liquid saturation enthalpy
GKONC	REAL	Thermal conduct. of the cont. phase without vapour
GKONV	REAL	Thermal conductivity of vapour
GLAGTS	INT.	Time-steps/cell
GLATVP	REAL	Latent heat of evaporation
GLHEAS	REAL	Latent heat of solidification
GLIQST	REAL	Liquidus temperature
GMWCON	REAL	Mol. Weight of continuous phase
GMWVAP	REAL	Mol. Weight of particle
GNUSS	REAL	Nusselt number
GPTYPE	INT.	Particle type
GSOLIN	REAL	Index for solid-fraction formula
GSOLST	REAL	Solidus temperature
GSTOCH	BOOL	Switch of stochastic turbulence model
GSTPRE	REAL	Saturation pressure of vapour
GSURPR	BOOL	Switch for pressure gradient effects
GVPAST	REAL	Saturation temperature of vapour

B.2.2 GENTRA Group 2: Boundary conditions

Variable	Type	Meaning
GINFIL	CHAR	Name of the file for particle inlet condition
GINSYS	INT.	Co-ordinate system for particle inlet condition
GPOROS	REAL	Threshold for obstacle porosity
GWALLC	NT.	Wall type
GWREST	REAL	Restitution coefficient of wall

B.2.3 GENTRA Group 3: Numerical controls

Variable	Type	Meaning
GDTMAX	REAL	Maximum Lagrangian time-step size
GDTRCT	REAL	Minimum particle diameter allowed
GLNRLX	REAL	Relaxation factor for sources of continuous phase
GRTFRC	REAL	Time step size multiplier
GSTEMX	INT.	Maximum number of time-steps
GSWEP1	INT.	1st GENTRA sweep
GSWEPF	INT.	Sweep frequency for GENTRA
GTIMMX	REAL	Flight timeout

B.2.4 GENTRA Group 4: Output controls

Name	Type	Meaning
GH1STC	CHAR	ID of individual history file
GHFILE	CHAR	Name of global history file
GOUTFR	INT.	Frequency (time-steps) for output
GRESTI	INT.	Cell-residence-time calculation
GRSFIL	CHAR	Name of particle restart file
GSWOUT	INT.	Frequency of writing output to screen
GT1STC	CHAR	ID of individual trajectory file
NGWEND	INT.	Last trajectory to write
NGWINT	INT.	Interval of writing trajectories
NGWSTR	INT.	First trajectory to write

Appendix C. List of GENTRA FORTRAN variables

The main GENTRA variables are listed in this Appendix. These variables are available through the `COMMON` blocks in the file `TRACMN`, a copy of which can be found in the `d_gentra` directory.

In the tables below, the numbers in square brackets indicate the built-in default value of the variable.

Additionally, all the GENTRA-PIL variables, listed in Appendix B, are also available in FORTRAN, and are automatically assigned the value specified for them in the Q1 file.

(Variables in *italics* **should not be modified** by the user.)

C.1 Variables for continuous phase

Name	Type	Meaning
CPVAPO	REAL	Cp of vapour
DENGAS	REAL	Density of the continuous phase
GASPRE	REAL	Pressure of the continuous phase
GCONGS	REAL	Vapour mass fraction
GCPGAS	REAL	Cp of cont. phase-vapour mixture
GEDLIF	REAL	Eddy life time
GEPSIL	REAL	Local dissipation rate of turbulence kinetic energy
GKINET	REAL	Local turbulence kinetic energy
GLENGT	REAL	Turbulence length scale
GSENUL	REAL	Laminar viscosity of the continuous phase
GVFLOW	REAL	Magnitude of velocity of cont. phase
HEAT	INT.	Index of energy source
PRINDX	INT.	Property index Threshold for solid
PROPS	INT.	Index of properties for cont. phase
RESMET	BOOL	Cal. of cont. phase has met the residual criterion
REST	INT.	Index of particle residence time
TEMGAS	REAL	Temperature of the continuous phase
THRMKC	REAL	Thermal conduct. of the cont. phase without vapour
TSOLVE	BOOL	Switch for solving particle energy equation
UCDASH	REAL	Vel. fluctuation of the cont. phase in Cart. system
UCGASN	REAL	Velocity of the continuous phase in Cartesian system
UPGASN	REAL	Velocity of the continuous phase in polar system
VAPO	INT.	Index of vapour concentration
VCDASH	REAL	Vel. fluctuation of the cont. phase in Cart. system
VCGASN	REAL	Velocity of the continuous phase in Cartesian system
VPGASN	REAL	Velocity of the continuous phase in polar system
WCDASH	REAL	Vel. fluctuation of the cont. phase in Cart. system
WCGASN	REAL	Velocity of the continuous phase in Cartesian system

C.2 Variables for particle phase

Name	Type	Meaning
DIAMAX	REAL	Maximum particle diameter
DIAMIN	REAL	Minimum particle diameter
DIPARN	REAL	New particle diameter
DIPARO	REAL	Old particle diameter
EPS	REAL	Restitution coefficient
GCPPAR	REAL	Cp of particle
GDT	REAL	Lagrangian time step size

<i>GEDTIM</i>	REAL	Traverse time for particle through eddy
<i>GHCSAA</i>	REAL	Coefficient in particle energy equation
<i>GHCSBB</i>	REAL	Coefficient in particle energy equation
<i>GHCSCC</i>	REAL	Source in particle energy equation
<i>GMCSAA</i>	REAL	Coefficient in particle mass equation
<i>GMCSBB</i>	REAL	Coefficient in particle mass equation
<i>GMSCC</i>	REAL	Source in particle mass equation
<i>GMINDX</i>	REAL	Index of solid fraction formula
<i>GNUSLT</i>	REAL	Nusselt number
<i>GPRYVS</i>	REAL	Vapour mass fraction under saturation condition
<i>GTIMED</i>	REAL	Total particle-eddy interaction time
<i>GTLIQD</i>	REAL	Liquidus temperature
<i>GTSOLD</i>	REAL	Solidus temperature
<i>GVCSAA</i>	REAL	Coefficient in particle momentum equation
<i>GVCSBB</i>	REAL	Coefficient in particle momentum equation
<i>GVCSCX</i>	REAL	Source in particle momentum equation
<i>GVSCSY</i>	REAL	Source in particle momentum equation
<i>GVSCSZ</i>	REAL	Source in particle momentum equation
<i>GVPART</i>	REAL	Magnitude of particle velocity
<i>HFGLIQ</i>	REAL	Latent heat of evaporation
<i>IP</i>	INT.	ID of the current particle
<i>IUPARN</i>	INT.	New index of particle containing momentum cell
<i>IUPARO</i>	INT.	Old index of particle containing momentum cell
<i>IVPARN</i>	INT.	New index of particle containing momentum cell
<i>IVPARO</i>	INT.	Old index of particle containing momentum cell
<i>IWPARN</i>	INT.	New index of particle containing momentum cell
<i>IWPARO</i>	INT.	Old index of particle containing momentum cell
<i>IXPARN</i>	INT.	New index of particle containing cell
<i>IXPARO</i>	INT.	Old index of particle containing cell
<i>IYPARN</i>	INT.	New index of particle containing cell
<i>IYPARO</i>	INT.	Old index of particle containing cell
<i>IZPARN</i>	INT.	New index of particle containing cell
<i>IZPARO</i>	INT.	Old index of particle containing cell
<i>KILPAR</i>	BOOL	Current particle is killed
<i>LABPAR</i>	INT.	Particle ID (internal use only)
<i>LASTF</i>	INT.	Last F-array address used
<i>LSTLAB</i>	INT.	ID of last particle
<i>MASS</i>	INT.	Index of mass source
<i>MOMX</i>	INT.	Index of X-momentum source
<i>MOMY</i>	INT.	Index of Y-momentum source
<i>MOMZ</i>	INT.	Index of Z-momentum source
<i>NPORTS</i>	INT.	Number of parcels introduced in the current Eulerian time step
<i>NTRACK</i>	INT.	Total number of parcels in the domain
<i>PARNUM</i>	REAL	Number of particles in the current parcel
<i>PMASSN</i>	REAL	New parcel mass
<i>PMASSO</i>	REAL	Old parcel mass
<i>PRVLIN</i>	REAL	Internal variable for particle init. condition
<i>RELVEC</i>	REAL	Magnitude of relative velocity (slip velocity)
<i>REYNOL</i>	REAL	Particle Reynolds number
<i>ROLIQD</i>	REAL	Liquid density of particle
<i>ROPARN</i>	REAL	New particle density
<i>ROPARO</i>	REAL	Old particle density
<i>ROSOLD</i>	REAL	Solid density of particle
<i>ROTCOO</i>	BOOL	Simulation is in rotating co-ordinate system
<i>SATPRS</i>	REAL	Vapour saturation pressure
<i>SOLFR0</i>	REAL	Initial particle solid-fraction

<i>SOLFRN</i>	REAL	New particle solid fraction
<i>SOLFRO</i>	REAL	Old particle solid fraction
<i>SOLIDF</i>	BOOL	Switch for solid./melt.
<i>SOLLAT</i>	REAL	Latent heat of solidification
<i>SPALD</i>	REAL	Spalding number
<i>STARAT</i>	REAL	Velocity criterion for particle stagnation
<i>THRMKV</i>	REAL	Thermal conduct. of vapour
<i>TPARTN</i>	REAL	New particle temperature
<i>TPARTO</i>	REAL	Old particle temperature
<i>TUOFF</i>	BOOL	Turning off turb. stochastic model (Internal use)
<i>UCNDRG</i>	REAL	Internal variable for particle momentum calculation
<i>UCPARN</i>	REAL	New particle velocity in Cartesian system
<i>UCPARO</i>	REAL	Old particle velocity in Cartesian system
<i>UPPARN</i>	REAL	New particle velocity in polar system
<i>UPPARO</i>	REAL	Old particle velocity in polar system
<i>VAPSOL</i>	BOOL	Flag for solving vapour concentration
<i>VCNDRG</i>	REAL	Internal variable for particle momentum calculation
<i>VCPARN</i>	REAL	New particle velocity in Cartesian system
<i>VCPARO</i>	REAL	Old particle velocity in Cartesian system
<i>VPPARN</i>	REAL	New particle velocity in polar system
<i>VPPARO</i>	REAL	Old particle velocity in polar system
<i>WCNDRG</i>	REAL	Internal variable for particle momentum calculation
<i>WCPARN</i>	REAL	New particle velocity in Cartesian system
<i>WCPARO</i>	REAL	Old particle velocity in Cartesian system
<i>WPGASN</i>	REAL	Velocity of the continuous phase in polar system
<i>WPPARN</i>	REAL	New particle velocity in polar system
<i>WPPARO</i>	REAL	Old particle velocity in polar system
<i>XCPARN</i>	REAL	New particle position in Cartesian system
<i>XCPARO</i>	REAL	Old particle position in Cartesian system
<i>XPPARN</i>	REAL	New particle position in polar system
<i>XPPARO</i>	REAL	Old particle position in polar system
<i>YCPARN</i>	REAL	New particle position in Cartesian system
<i>YCPARO</i>	REAL	Old particle position in Cartesian system
<i>YPPARN</i>	REAL	New particle position in polar system
<i>YPPARO</i>	REAL	Old particle position in polar system
<i>ZCPARN</i>	REAL	New particle position in Cartesian system
<i>ZCPARO</i>	REAL	Old particle position in Cartesian system
<i>ZPPARN</i>	REAL	New particle position in polar system
<i>ZPPARO</i>	REAL	Old particle position in polar system

C.3 Printout variables

Name	Type	Meaning
<i>LUFAT</i>	INT.	Logical unit for GENTRA fatal error
<i>LUHIS</i>	INT.	Logical unit for GENTRA global history file
<i>LUPRO</i>	INT.	Logical unit for screen output
<i>LUTRA</i>	INT.	Logical unit for PHOTON use file
<i>LUWAR</i>	INT.	Logical unit for GENTRA warning message
<i>TRCOLO</i>	INT.	Colour index of trajectory
<i>TRDASH</i>	INT.	line style index of trajectory

C.4 Auxiliary variables

Name	Type	Meaning
ANODAL	REAL	Internal variable
AXISYM	BOOL	Axi-symmetric case
AXIXRY	BOOL	Internal variable
AXIXRZ	BOOL	Internal variable
AXIYRX	BOOL	Internal variable
AXIYRZ	BOOL	Internal variable
AXIZRX	BOOL	Internal variable
AXIZRY	BOOL	Internal variable
BNODAL	REAL	Internal variable
CCHLIM	REAL	Internal variable
CCLLIM	REAL	Internal variable
CCNMAX	REAL	Internal variable
CCNMIN	REAL	Internal variable
CELMIN	REAL	Internal variable
CENTRA	REAL	Internal variable
CHARVL	REAL	Characteristic velocity
CNODAL	REAL	Internal variable
DBGLEV	INT.	For internal debugging only
DBGPAR	INT.	For internal debugging only
DBGSWP	INT.	For internal debugging only
DIHLIM	REAL	Internal variable
DILLIM	REAL	Internal variable
DISAX	REAL	Internal variable
DISAY	REAL	Internal variable
DISAZ	REAL	Internal variable
DISBX	REAL	Internal variable
DISBY	REAL	Internal variable
DISBZ	REAL	Internal variable
DNODAL	REAL	Internal variable
ENODAL	REAL	Internal variable
FACEVS	REAL	Internal variable
FNODAL	REAL	Internal variable
FULCYC	BOOL	The domain covers full cycle
FVISIT	BOOL	Internal variable
GBUOYA	BOOL	PIL variable
GCARTE	BOOL	Cartesian system
GCPCON	REAL	PIL variable
GCPLIQ	REAL	PIL variable
GCPSOL	REAL	PIL variable
GCPVAP	REAL	PIL variable
GDRAG	REAL	PIL variable
GDTMAX	REAL	PIL variable
GDTMIN	REAL	Minimum time step size allowed
GDTRCT	REAL	PIL variable
GFASWP	INT.	First actual GENTRA sweep
GGRAX	REAL	PIL variable
GGRAY	REAL	PIL variable
GGRAZ	REAL	PIL variable
GH1STC	CHAR	PIL variable
GHFILE	CHAR	PIL variable
GHLIQD	REAL	PIL variable
GINFIL	CHAR	PIL variable
GKONC	REAL	PIL variable

GKONV	REAL	PIL variable
GLAGTS	INT.	PIL variable
GLATVP	REAL	PIL variable
GLHEAS	REAL	PIL variable
GLIQST	REAL	PIL variable
GMWCON	REAL	PIL variable
GMWVAP	REAL	PIL variable
GNODAL	REAL	Internal variable
GNUSS	REAL	PIL variable
GOUTFR	INT.	PIL variable
GPOLAR	BOOL	Polar system
GPOROS	REAL	PIL variable
GPTYPE	INT.	PIL variable
GRESTI	INT.	PIL variable
GRSTRT	CHAR	PIL variable GRSFIL
GRTFRC	REAL	PIL variable
GSOLIN	REAL	PIL variable
GSOLST	REAL	PIL variable
GSTEMX	INT.	PIL variable
GSTOCH	BOOL	PIL variable
GSTPRE	REAL	PIL variable
GSURPR	BOOL	PIL variable
GSWEP1	INT.	PIL variable
GSWEPF	INT.	PIL variable
GSWOUT	INT.	PIL variable
GT1STC	CHAR	PIL variable
GTIMMX	REAL	PIL variable
GVAPST	REAL	PIL variable
GWALLC	INT.	PIL variable
GWREST	REAL	PIL variable
GXCYCL	BOOL	Cyclic boundary condition
HNODAL	REAL	Internal variable
IBODRY	INT.	Internal variable
IBONCF	INT.	Internal variable
IGAXI	INT.	Internal variable
ILOC0	INT.	Internal variable
INTLEV	INT.	For internal debugging only
IPRDIA	INT.	Internal variable
IPRLAB	INT.	Internal variable
IPRLIQ	INT.	Internal variable
IPRNUM	INT.	Internal variable
IPRSOF	INT.	Internal variable
IPRSOL	INT.	Internal variable
IPRSTN	INT.	Internal variable
IPRT0	INT.	Internal variable
IPRTEM	INT.	Internal variable
IPRVEL	INT.	Internal variable
ITEMIN	INT.	Internal variable
IVARBL	INT.	Internal variable
JCOUNT	INT.	Internal variable
JGAXI	INT.	Internal variable
JTEM1	INT.	Internal variable
JUCRT	INT.	Internal variable
JVCRT	INT.	Internal variable
JWCRT	INT.	Internal variable
KGAXI	INT.	Internal variable
LSTSWP	BOOL	Flag for PHOENICS last sweep

<i>LUEND</i>	INT.	Internal variable
<i>NFACE</i>	INT.	Internal variable
<i>NGWEND</i>	INT.	PIL variable
<i>NGWINT</i>	INT.	PIL variable
<i>NGWSTR</i>	INT.	PIL variable
<i>PI</i>	REAL	3.1415926
<i>POLTRC</i>	BOOL	Tracking in polar system
<i>SUBEDY</i>	BOOL	Internal variable
<i>TCHLIM</i>	REAL	Internal variable
<i>TCLLIM</i>	REAL	Internal variable
<i>TCNMAX</i>	REAL	Internal variable
<i>TCNMIN</i>	REAL	Internal variable
<i>TCONST</i>	BOOL	Internal variable
<i>TPHLIM</i>	REAL	Internal variable
<i>TPLLIM</i>	REAL	Internal variable
<i>TPRMAX</i>	REAL	Internal variable
<i>TPRMIN</i>	REAL	Internal variable
<i>UA</i>	REAL	Internal variable
<i>UB</i>	REAL	Internal variable
<i>VA</i>	REAL	Internal variable
<i>VB</i>	REAL	Internal variable
<i>VPHLIM</i>	REAL	Internal variable
<i>VPLLIM</i>	REAL	Internal variable
<i>VPRMAX</i>	REAL	Internal variable
<i>VPRMIN</i>	REAL	Internal variable
<i>WA</i>	REAL	Internal variable
<i>WB</i>	REAL	Internal variable
<i>XCFACE</i>	REAL	Internal variable
<i>XLASTM</i>	REAL	Internal variable
<i>YLASTM</i>	REAL	Internal variable
<i>ZLASTM</i>	REAL	Internal variable

Appendix D. List of Run-Time Errors

D.1 Introduction

All the errors reported by GENTRA-EARTH at runtime have an identification number. This section contains a compilation of the errors, with explanations and, where appropriate, avoidance instructions.

This list is also available interactively through the menu. See Section 2.5 for instructions on how to access it. If your version of GENTRA is more recent than the one described in this manual, you should also refer to menu for an updated list of errors.

Section 2.5 of this Guide provides additional information on how errors are classified and handled by GENTRA.

D.2 Warning messages

Warning number 001:

Stochastic turbulence model active but no KE or EP

Explanation:

The stochastic model for the dispersion of particles owing to turbulence was activated in the GENTRA menu, but KE (the continuous-phase turbulence-kinetic-energy) or EP (its rate of dissipation) are not stored in the Q1 file. The stochastic turbulence model is automatically deactivated by GENTRA.

Remedy:

Activate the storage or solution of KE (and/or EP) in the Q1 file, through STORE, SOLVE or SOLUTN; or, if using a menu system for problem set-up, choose a turbulence model that uses KE and EP.

Warning number 002:

Stochastic turbulence model not available for stubborn particles

Explanation:

The stochastic model for the dispersion of particles owing to turbulence was activated in the GENTRA menu, but the particle type does not allow it. The stochastic turbulence model is automatically deactivated by GENTRA.

Warning number 003:

Particle removal is the only wall condition available for lazy and stubborn particles

Explanation:

On hitting a wall or obstacle, the lazy and stubborn particles are always removed from the computational domain. Other wall effects are not available for these particles.

Warning number 004:***GENTRA first sweep less than FSWEEP***

Explanation:

The user has specified a GENTRA first sweep that is less than FSWEEP (the EARTH first sweep). The GENTRA first sweep is reset automatically to FSWEEP.

Warning number 005:***Particle <ip> initially in wrong position******Tracking for the particle skipped***

Explanation:

The initial position of a particle (identified by its number <ip>) was initially an incorrect one (e.g., outside the computational domain or in a blocked region). The particle was skipped.

Remedy:

Specify a correct initial position in the inlet-data table.

Warning number 006:***Error reading inlet data in line:***

<line>

Not enough or too many data items for

this particle:

Read- <read> Needed- <needed>

The data line has been ignored

Explanation:

A inlet-data line had a number of data items different from that required; the line was ignored. The <line>, the number of data-items <read> and the number of data-items <needed> are displayed.

The number of inlet data-items needed for each particle varies from case to case; a suitable heading for the table is provided for your guidance in the Q1 file by the GENTRA menu.

Warning number 007:**Error reading inlet data in line:****<line>****Line discarded**

Explanation:

A inlet-data line could not be read correctly. The likely causes of this warning are: (1) A character was used instead of a number (e.g. letter O instead of number zero); (2) A comment line was included in the table, but without an asterisk.

Warning number 008:**Inlet data from Q1 but no****<END-GENTRA-INLET> mark. Mark assumed**

Explanation:

When reading inlet data from the Q1 file, the <END-GENTRA-INLET> mark, which flags the end of the inlet-data table, was not found. The mark was assumed and the calculation continues.

Warning number 009:**Variable out of range****Variable: <var>****Value: <value>****Valid range: <range>**

Explanation:

Variable <var> was supplied a <value> which is not within the permissible <range>.

Warning number 010:**FALSDT relaxation not available for <source name>****The source is left unrelaxed**

Explanation:

False-time-step (FALSDT) relaxation was specified for the inter-phase source indicated in the warning message. Since only linear relaxation (LINRLX) is allowed for the sources, the source in question was left unrelaxed by GENTRA.

D.3 Error messages

Error number 301:***Mass transfer active but MASS not STOREd***

Explanation:

Mass transfer between particles and gas was activated in the GENTRA menu, but the user has not STOREd the variable MASS in the Q1 file.

Remedy:

STORE(MASS) in the Q1 file. (This is done automatically by the GENTRA menu when the particle type chosen by the user entails mass transfer)

Error number 302:***Invalid particle type (GPTYPE)***

Explanation:

An invalid particle type was specified through the variable PIL variable GPTYPE.

Remedy:

See the information on GPTYPE in the GENTRA User Guide (or through the menu) for a list of available particle types.

Error number 303:***NCRT must be 1***

Explanation:

In BFC cases, the PIL variable NCRT (the sweep frequency for the calculation of the Cartesian components) must be 1.

Remedy:

Set NCRT=1 in the Q1 file; then re-run the SATELLITE and EARTH.

Error number 305:***GENIUS called but property not set ?******Property: <prop>***

Explanation:

A GRNDn flag was used for the particle property <prop>, indicating that its value was to be computed in the FORTRAN subroutine GENIUS. However, no value for the property was supplied there.

Remedy:

Insert the appropriate coding in GENIUS, and then re-compile and re-link.

Error number 306:***Inlet data from Q1 but no******<GENTRA-INLET-DATA> mark***

Explanation:

The user has specified that the Q1 file is the file where the inlet data table is to be found, but GENTRA could not find the <GENTRA-INLET-DATA> mark.

Remedy:

If there is no <GENTRA-INLET-DATA> mark at the beginning of your data, insert it. If there is, check that: the line starts from the third column of the Q1 file; the mark is separated from other text in the line by blank spaces; there is not an asterisk in the same line.

Error number 307:***F-Array too small for particle data******Current size: <size>. Increase !***

Explanation:

GENTRA stores the particle-inlet data in the F-array (the central storage array of EARTH). The message is produced when there is not enough F-array space to store further particles. <size> is the current F-array size

Remedy:

You can increase the F-array dimension by changing the parameter `NFDIM` in the `MAIN PROGRAM` of EARTH. (In the GENTRA version of EARTH, the `MAIN PROGRAM` is in the file GENTRA.) The storage needs for GENTRA are case-dependent, but the maximum requirement is 13 F-array positions per particle.

Note that recompilation of the file GENTRA and re-linking of the EARTH executable is needed after this change.

Error number 308:***No inlet data found !***

Explanation:

GENTRA could not find any inlet data for particles.

Remedy:

Check the name of inlet data file supplied to GENTRA (ie, the variable `GENFIL` in the Q1 file). If the file name is Q1, then your data should be inserted as comment lines in the Q1 file, between the marks <GENTRA-INLET-DATA> and <END-GENTRA-INLET>.

Error number 309:***GENTRA is not unlocked !***

Explanation:

The password (also called ID string) that authorises the EARTH run does not allow the execution of GENTRA.

Remedy:

Possible causes are:- (1) your licence type does not include GENTRA; (2) your GENTRA licence has expired; (3) you have not inserted the CHAM-supplied ID string in the CONFIG file.

In cases (1) and (2), please contact the Sales Department at CHAM. In case (3), please refer to the PHOENICS Installation Manual (CHAM TR/110) for instructions, and contact CHAM if in doubt.

Error number 310:

***Exit/symmetry patch type must be EAST,
WEST, NORTH, SOUTH, HIGH or LOW only.***

Offending PATCH: <patchname>

Explanation:

One of the symmetry or exit patches declared by the user has a patch type (such as CELL, VOLUME, LWALL, etc) which is not of the 'area' type. <patchname> is the name of the patch causing the error.

Remedy:

Change, in the Q1 file, the patch type to one of the allowed types (listed above). (The help facility in the GENTRA menu system provides advice on patch types.) The SATELLITE must be re-run after changing the Q1 file, but the GENTRA menu does not need to be loaded again.

Error number 311:

Variable out of range

Variable: <var>

Value: <value>

Valid range: <range>

Explanation:

Variable <var> was supplied a <value> which is not within the permissible <range>

Error number 312:

GENTRA cannot be used for PARABolic flows

Explanation:

GENTRA cannot be used in conjunction with the parabolic option of PHOENICS (activated by PARAB=T)

Remedy:

Parabolic flows can also be solved as elliptic by supplying outlet boundary conditions and setting PARAB=F.

D.4 Internal errors

Errors with numbers greater than 600 are internal errors. Internal errors should be reported to CHAM via the User Support Team.

Please e-mail the Q1 causing the error to CHAM, and report as many details as you can; further details might be requested by CHAM upon notification of the error.

e-mail: support@cham.co.uk

Appendix E. Listing of the Q1 File for the Example

The worked example is based on library case B534. This is a listing of case B534 after passing through the steps described in Chapter 2.

```
TALK=T;RUN( 1, 1)
```

```
*****
```

```
Q1 created by VDI menu, Version 3.5, Date 12/11/02
```

```
CPVNAM=VDI;SPPNAM=Core
```

```
*****
```

```
Echo DISPLAY / USE settings
```

```
PHOTON USE
```

```
P
```

```
use patgeo
```

```
msg Geometry
```

```
vec x 1 sh
```

```
MSG Velocity vectors
```

```
msg
```

```
msg Press return to plot pressure contours
```

```
pause
```

```
cont p1 x 1 fil;.001
```

```
msg
```

```
msg Press return to plot streamlines
```

```
pause
```

```
clear
```

```
stream sh
```

```
x 1
```

```
y
```

```
posit
```

```
3
```

```
0.51268E+02 0.20453E+04 CR
```

```
0.38451E+02 0.19150E+04 CR
```

```
0.44859E+02 0.17847E+04 CR
```

```
0.76901E+02 0.16740E+04 CR
```

```
0.57676E+02 0.15502E+04 CR
```

```
0.57676E+02 0.14200E+04 CR
```

```
0.51268E+02 0.13548E+04 CR
```

```
0.11792E+04 0.12571E+04 t
```

```
exit
```

```
use patgeo
```

```
msg
```

```
msg Type e to End
```

```
ENDUSE
```

```
DISPLAY
```

The incompressible, single-phase flow of water through a fully-open axi-symmetric ball valve is solved. The pipe-work considered is 2 m in length; the radius at inlet is 0.15 m; it diminishes to a minimum of 0.09 m in front of the ball; and the maximum radius is 0.16 m.

A plug profile of axial velocity is prescribed at the inlet, and a fixed-pressure condition is employed at outlet. Wall friction is activated along the boundary of the ball, and along the pipe wall. A fixed turbulent kinematic viscosity is set to 100 times the laminar value (the Reynolds number is of order $1.0E5$).

ENDDIS

```
*****
IRUNN      =          1 ;LIBREF =          1
*****
```

Group 1. Run Title

```
TEXTFLOW THROUGH A BALL VALVE :          B534 )
*****
```

Group 2. Transience

```
STEADY     =          T
*****
```

Groups 3, 4, 5 Grid Information

```
* Overall number of cells, RSET(M,NX,NY,NZ,tolerance)
RSET(M,1,12,30)
```

```
* Set overall domain extent:
```

```
*          xulast yvlast zwlast
          name
```

```
* Set overall domain extent:
```

```
*          xulast yvlast zwlast
          name
```

```
XSI= 1.000000E+00; YSI= 1.000000E+00; ZSI= 1.000000E+00
```

```
RSET(D,CHAM      )
```

```
* Set objects: x0          y0          z0
```

```
*          dx          dy          dz
          name
```

```
XPO= 0.000000E+00; YPO= 0.000000E+00; ZPO= 3.333333E-01
```

```
XSI= 1.000000E+00; YSI= 8.333337E-02; ZSI= 5.666666E-01
```

```
RSET(B,CMP0      )
```

```
XPO= 0.000000E+00; YPO= 0.000000E+00; ZPO= 0.000000E+00
```

```
XSI= 1.000000E+00; YSI= 1.000000E+00; ZSI= 0.000000E+00
```

```
RSET(B,INLET     )
```

```
XPO= 0.000000E+00; YPO= 0.000000E+00; ZPO= 1.000000E+00
```

```
XSI= 1.000000E+00; YSI= 1.000000E+00; ZSI= 0.000000E+00
```

```
RSET(B,OUTLET    )
```

```
XPO= 0.000000E+00; YPO= 1.000000E+00; ZPO= 0.000000E+00
```

```
XSI= 1.000000E+00; YSI= 0.000000E+00; ZSI= 1.000000E+00
```

```
RSET(B,WFUN      )
```

```
XPO= 0.000000E+00; YPO= 8.333337E-02; ZPO= 3.333333E-01
```

```
XSI= 1.000000E+00; YSI= 0.000000E+00; ZSI= 5.666666E-01
```

```
RSET(B,VALVEWLL)
```

```
*****
```

Group 6. Body-Fitted coordinates

```
BFC=T
```

```
READCO(grid4)
```

```
*****
```

```
NONORT     =          T
```

```
NCRT       =          1
*****
```

Group 7. Variables: STOREd,SOLVEd,NAMED

```
ONEPHS     =          T
```

```
* Non-default variable names
```

```

NAME(143) =REST ; NAME(144) =MOMZ
NAME(145) =MOMY ; NAME(146) =NPOR
NAME(147) =VPOR ; NAME(148) =WCRT
NAME(149) =VCRT ; NAME(150) =UCRT
  * Solved variables list
SOLVE(P1 ,V1 ,W1 )
  * Stored variables list
STORE(UCRT,VCRT,WCRT,VPOR,NPOR,MOMY,MOMZ,REST)
  * Additional solver options
SOLUTN(P1 ,Y,Y,Y,N,N,N)

*****
Group 8. Terms & Devices
DIFCUT = 0.000000E+00
*****

Group 9. Properties
RHO1 = 1.000000E+03
ENUL = 1.000000E-06
CP1 = 1.000000E+00
ENUT = 1.000000E-04
*****

Group 10. Inter-Phase Transfer Processes
*****

Group 11. Initialise Var/Porosity Fields
FIINIT(W1 ) = 2.000000E+00 ;FIINIT(NPOR) = 1.000000E+00
FIINIT(VPOR) = 1.000000E+00 ;FIINIT(WCRT) = 1.001000E-10
FIINIT(VCRT) = 1.001000E-10 ;FIINIT(UCRT) = 1.001000E-10
No PATCHes used for this Group

INIADD = F
*****

Group 12. Convection and diffusion adjustments
No PATCHes used for this Group
*****

Group 13. Boundary & Special Sources

INLET (INLET ,LOW ,2,0,0,0,0,0,1,1)
VALUE (INLET ,P1 , 2.000000E+03)
VALUE (INLET ,W1 , 2.000000E+00)

PATCH (GENPAT ,CELL ,0,0,0,0,0,0,1,1)
COVAL (GENPAT ,V1 , FIXFLU , GRND )
COVAL (GENPAT ,W1 , FIXFLU , GRND )

*****

Group 14. Downstream Pressure For PARAB
*****

Group 15. Terminate Sweeps
LSWEEP = 200
RESFAC = 1.000000E-03
*****

Group 16. Terminate Iterations
*****

Group 17. Relaxation
RELAX(P1 ,LINRLX, 2.000000E-01)

```

```

RELAX(V1 ,FALSDT, 3.333333E-03)
RELAX(W1 ,FALSDT, 3.333333E-03)
RELAX(MOMZ,LINRLX, 7.000000E-01)
RELAX(MOMY,LINRLX, 7.000000E-01)
*****
Group 18. Limits
VARMAX(V1 ) = 1.000000E+06 ;VARMIN(V1 ) = -1.000000E+06
VARMAX(W1 ) = 1.000000E+06 ;VARMIN(W1 ) = -1.000000E+06
*****
Group 19. EARTH Calls To GROUND Station
USEGRD = T ;USEGRX = T
L($G001
GENTR = T
*-----
* GENTRA GROUP 1: Particle physics
*-----
* Particle type - 30
GPTYPE = 30
* Gravity components in GENTRA Cartesian system
GGRAX = 0.000000E+00 ;GGRAY = 0.000000E+00
GGRAZ = 9.800000E+00
* Buoyancy forces
GBUOYA = F ;GSURPR = F
* Stochastic model of turbulence
GSTOCH = F
* Data for isothermal particles
GDRAG = GRND1
*-----
* GENTRA GROUP 2: Boundary conditions for particles
*-----
* Inlet-data file-name
GINFIL = 'Q1'
<GENTRA-INLET-DATA>
*__YP__ZP__VP__WP__DI_LDEN_MDOT_(NUM)
0.01 0.0 0 1 0.001 500.0 1.0E-5
0.04 0.0 0 2 0.0001 1000.0 1.0E-5
0.07 0.0 0 3 0.0015 1000.0 1.0E-5
0.10 0.0 0 0.5 0.002 1000.0 1.0E-5
0.13 0.0 0 1 0.001 1500.0 1.0E-5
<END-GENTRA-INLET>
* Wall treatment, and rest coefficient if appropriate
GWALLC = 3
GWREST = 7.500000E-01
* Porosity threshold
GPOROS = 0.000000E+00
*-----
* GENTRA GROUP 3: Numerical controls
*-----
* 1st GENTRA sweep; frequency of calls
GSWEP1 = 190 ;GSWEPF = 1
* Maximum Lagrangian time-step; time step size multiplier
GDTMAX = 1.000000E+00 ;GRTFRC = 7.000000E-01
* Min # of t-steps per cell; max # of t-steps; timeout
GLAGTS = 5 ;GSTEMX = -100
GTIMMX = 1.000000E+01
*-----

```

```

* GENTRA GROUP 4: Output controls
*-----
* Restart-file, history-file and frequency for output
GRSFIL  ='NONE'
GHFILE  ='GHIS'
GOUTFR  =      1
* The identifier of the individual history and
  trajectory files
GH1STC  ='NONE'
GT1STC  ='T'
* The first, last particles and the interval for
  writing history and trajectory files
NGWSTR  =      1 ;NGWEND =      5 ;NGWINT =      1
GSWOUT  =      1
* Particle number for residence-time calculation
GRESTI  =      2
L(GENSET
*****
  Group 20. Preliminary Printout
ECHO    =      T
*****
  Group 21. Print-out of Variables
*****
  Group 22. Monitor Print-Out
IXMON   =      1 ;IYMON   =      2 ;IZMON   =      20
NPRMON  = 100000
NPRMNT  =      1
TSTSWP  =     -1
*****
  Group 23. Field Print-Out & Plot Control
NPRINT  = 100000
NYPRIN  =      2
NZPRIN  =      5
NPLT    =      2
ISWPRF  =      1 ;ISWPRL = 100000

PATCH (DOMAIN ,CONTUR,1,1,1,12,1,30,1,1)
PLOT(DOMAIN ,P1 , 0.000000E+00, 1.500000E+01)

PATCH (INNER ,PROFIL,1,1,2,2,1,30,1,1)
PLOT(INNER ,W1 , 0.000000E+00, 0.000000E+00)

PATCH (OUTER ,PROFIL,1,1,12,12,1,30,1,1)
PLOT(OUTER ,W1 , 0.000000E+00, 0.000000E+00)

PATCH (FRONT ,PROFIL,1,1,2,12,10,10,1,1)
PLOT(FRONT ,P1 , 0.000000E+00, 0.000000E+00)
PLOT(FRONT ,V1 , 0.000000E+00, 0.000000E+00)
PLOT(FRONT ,W1 , 0.000000E+00, 0.000000E+00)

PATCH (BACK ,PROFIL,1,1,2,12,28,28,1,1)
PLOT(BACK ,P1 , 0.000000E+00, 0.000000E+00)
PLOT(BACK ,V1 , 0.000000E+00, 0.000000E+00)
PLOT(BACK ,W1 , 0.000000E+00, 0.000000E+00)
*****
  Group 24. Dumps For Restarts

```

```

GVVIEW(P,-1.000000E+00,0.000000E+00,0.000000E+00)
GVVIEW(UP,0.000000E+00,1.000000E+00,0.000000E+00)

> DOM,      SIZE,      1.000000E+00, 1.200000E+01, 3.000000E+01
> DOM,      MONIT,     1.000000E+00, 2.000000E+00, 2.000000E+01
> DOM,      SCALE,     1.000000E+00, 1.000000E+00, 1.000000E+00
> DOM,      SNAPSIZ,   1.000000E-02

> OBJ,      NAME,      CMP0
> OBJ,      POSITION,   0.000000E+00, 0.000000E+00, 1.000000E+01
> OBJ,      SIZE,      1.000000E+00, 1.000000E+00, 1.700000E+01
> OBJ,      CLIPART,   CMP0
> OBJ,      TYPE,      BLOCKAGE
> OBJ,      MATERIAL,  199

> OBJ,      NAME,      INLET
> OBJ,      POSITION,   0.000000E+00, 0.000000E+00, 0.000000E+00
> OBJ,      SIZE,      1.000000E+00, 1.200000E+01, 0.000000E+00
> OBJ,      CLIPART,   INLET
> OBJ,      TYPE,      USER_DEFINED

> OBJ,      NAME,      OUTLET
> OBJ,      POSITION,   0.000000E+00, 0.000000E+00, 3.000000E+01
> OBJ,      SIZE,      1.000000E+00, 1.200000E+01, 0.000000E+00
> OBJ,      CLIPART,   OUTLET
> OBJ,      TYPE,      OUTLET
> OBJ,      PRESSURE,   0.000000E+00
> OBJ,      TEMPERATURE, -1.026000E+04
> OBJ,      COEFFICIENT, 1.000000E+03
> OBJ,      VELOCITY,   0.000000E+00, 0.000000E+00, 2.000000E+00

> OBJ,      NAME,      WFUN
> OBJ,      POSITION,   0.000000E+00, 1.200000E+01, 0.000000E+00
> OBJ,      SIZE,      1.000000E+00, 0.000000E+00, 3.000000E+01
> OBJ,      CLIPART,   WFUN
> OBJ,      TYPE,      PLATE

> OBJ,      NAME,      VALVEWLL
> OBJ,      POSITION,   0.000000E+00, 1.000000E+00, 1.000000E+01
> OBJ,      SIZE,      1.000000E+00, 0.000000E+00, 1.700000E+01
> OBJ,      CLIPART,   VALVEWLL
> OBJ,      TYPE,      PLATE
> OBJ,      POROSITY,   0.000000E+00
> OBJ,      SIDE,      HIGH
STOP

```

Appendix F. Contents of the GENTRA Input Library

Overview:

- Group 1: Lazy and stubborn particles
- Group 2: Particles in isothermal flow
- Group 3: Particles with heat transfer
- Group 4: Particles with solidification
- Group 5: Particles with mass transfer
- Group 6: Particle tracking with density calculation

Loading instructions:

To load a library case, click on **File, Load from Libraries**, enter the case number in the Library dialog box and click OK.

Group 1 - Lazy and stubborn particles

- G704: Tracers in pipe with bend (BFC=T,3D)
- G706: Beams in reaction turbine (BFC=T, LIBREF=525)

Group 2 - Particles in isothermal flow

- G200: Particles in backward-facing step (STM test)
- G201: Spray dryer (BFC=T)
- G204: Particles in radial impeller (BFC,rotating,LIBREF=424)
- G205: Particles through ball valve (BFC=T,LIBREF=534)
- G207: Rain in sample cup (CARTES=F,LIBREF=237)
- G209: Particles in 2D curved duct (BFC=T, CONJUGATE HEAT TRANSFER)

Group 3 - Particles with heat transfer

- G301: Particle heating in pipe with constant gas temperature and particle velocity (transient)
- G302: Heat-exchanging, 1-d, steady, $cp=a+bt$
- G303: Heat-exchanging, 1-d, transient, $cp=a+bt$

Group 4 - Particles with solidification

- G401: Solidifying, 1-d, transient, $m=3.0$
- G403: Solidifying, 1-d, transient, $l=l(t)$
- G405: Isothermal solidification (TRANSIENT).

Group 5 - Particles with mass transfer

- U502: Particle evaporating in pipe with constant gas temperature and particle velocity, but changing vapour concentration (particle temperature is also kept constant, TRANSIENT)
- U505: Evaporating particles in spray dryer (BFC)
- U506: Particles in 2D curved duct (BFC=T, CONJUGAT HEAT TRANSFER)
- U507: Particles in 2D channel (SOLVE H1)
- U508: Isothermal evaporation, constant prop's, steady

Group 6 - Particle tracking with density calculation

- G722: Oblique impingement of box in water

Appendix G. Listing of GENIUS

```

C
      SUBROUTINE GENTRA
C-----
-----C
C*
C*   This subroutine is part of the GENTRA particle-tracker option
C*   of PHOENICS
C
C-----
-----C
      INCLUDE '/phoenics/d_includ/satear'
      INCLUDE '/phoenics/d_includ/grdloc'
      INCLUDE '/phoenics/d_includ/satgrd'
      INCLUDE '/phoenics/d_includ/grdbfc'
      INCLUDE '/phoenics/d_includ/grdear'
      INCLUDE '/phoenics/d_includ/bfclear'
      INCLUDE '/phoenics/d_includ/tracmn'
      INCLUDE '/phoenics/d_includ/moncom'
      COMMON/GENI/IDUM1(10),NWOLE,IDUM2(31),NFTOT,IDUM3(2),LOOPZ,
1      IDUM4(14)
      COMMON/GENCHQ/CHQ(8)
      LOGICAL GENCAL,PSTLSW,QNE,QEQ
      CHARACTER*80 BUFF(3)
      INTEGER HEATZ
C.... ISWCNT is a safeguard for the end of time step
      SAVE GENCAL, PSTLSW, LGSWEP
C=====
=====
C
C   GROUP 1. Run title
C   =====
C      IF(IGR.EQ.1) THEN
C          * ----- SECTION 2 ----- GENTRA Preparation
C              IF(ISC.EQ.1) THEN
C                  CALL GENPRE
C                  GENCAL=.FALSE.
C                  PI=3.1415927
C                  IF(LG(10)) THEN
C                      DO 101 IS=1,8
101              CHQ(IS)=0.0
C                      ENDIF
C              * ----- SECTION 2 -----
C              ELSEIF(ISC.EQ.2) THEN
C
C....      NFTOT is the last used storage in F array
C              IPRT0=MAX0(NFTOT,NBFTOT,NF1TOT)
C.....      0 location for first particle
C              LASTF=IPRT0
C              NOTGXM= .NOT.(TSTSWP.EQ.12345.OR.TSTSWP.EQ.10001.OR.
+              TSTSWP.LT.0)
C              ENDIF
C
C   GROUP 9. Properties of the medium (or media)

```

```

C          =====
C      ELSEIF(IGR.EQ.9) THEN
C          * ----- SECTION 1: Density of phase 1 (DEN1)
C          IF(ISC.EQ.1.AND.QEQ(RHO1,GRND)) THEN
C              IF(LG(30).AND.ISTEP.GT.1) CALL FN2(DEN1,C1,RG(1),RHO2-
RG(1))
C
C              IF(STORE(VAPO).AND.STORE(DEN1).AND.
1          (STORE(JTEM1).OR.STORE(H1))) THEN
C....      Gas constant
C              FN2A=8314.0/GMWCON
C              FN2B=8314.0/GMWVAP-FN2A
C              L0FVAP=L0F(VAPO)
C              IF(STORE(JTEM1))L0FTEM=L0F(JTEM1)
C              IF(STORE(H1))L0FH1=L0F(H1)
C              L0FDEN=L0F(DEN1)
C              L0FPRE=L0F(P1)
C              IF(STORE(VPOR))L0FVPO=L0F(VPOR)
C              IF(STORE(PROPS))L0FPRP=L0F(PROPS)
C              DO 9010 J=1,NY
C                  DO 9010 I=1,NX
C                      JNYIM1=J+NY*(I-1)
C....      Is this is a blocked cell?
C                      CALL SUB2R(SOLREG,0.0,CHKBLK,1.1)
C                      IF(STORE(VPOR)) CHKBLK=F(L0FVPO+JNYIM1)
C                      IF(STORE(PROPS))SOLREG=F(L0FPRP+JNYIM1)
C                      IF(SOLREG.LT.REAL(PRINDX).AND.CHKBLK.GT.GPOROS) THEN
C....      the vapour mass fraction,
C                      VAPOUR=F(L0FVAP+JNYIM1)
C....      Find the local temperature,
C                      IF(STORE(JTEM1)) THEN
C                          CTEMPR=F(L0FTEM+JNYIM1)
C                      ELSEIF(STORE(H1)) THEN
C....      Currently this is only for constant Cp. The user
C      can
C              change it, so that Cp will be a function of
C      local
C              and vapour mass fraction. Iteration may be
C      needed for
C              that purpose.
C              CTEMPR=TMP1A+TMP1B*F(L0FH1+JNYIM1)
C              ENDIF
C....      the gas constant for the mixture
C              GASCOS=FN2A+FN2B*VAPOUR
C....      the pressure
C              PRESSR=F(L0FPRE+JNYIM1)
C....      and finally the density
C              F(L0FDEN+JNYIM1)=(PRESSR+PRESS0)/(GASCOS*CTEMPR)
C              ENDIF
C      9010      CONTINUE
C              ENDIF
C          * ----- SECTION 10: Temperature
C          ELSEIF(ISC.EQ.10.AND.INT(TMP1).EQ.INT(GRND)) THEN
C              IF(STORE(JTEM1).AND.SOLVE(H1)) THEN
C                  L0FTEM=L0F(JTEM1)
C                  L0FH1=L0F(H1)

```

```

        IF(STORE(VAPO)) L0FVAP=L0F(VAPO)
        DO 9110 J=1,NY
            DO 9110 I=1,NX
                JNYIM1=J+NY*(I-1)
                CENTHP=F(L0FH1+JNYIM1)
                CTEMPR=F(L0FTEM+JNYIM1)
                VAPOUR=0.0
                IF(STORE(VAPO)) VAPOUR=F(L0FVAP+JNYIM1)
                GCPGAS=(1.0-VAPOUR)*GPROPS(16, CTEMPR, GCPCON)+
+                VAPOUR*GPROPS(15, CTEMPR, GCPVAP)
                F(L0FTEM+JNYIM1)=GPROPS(6, CENTHP, GRND1)
9110          CONTINUE
            ENDIF
        ENDIF
C
        ELSEIF(IGR.EQ.11) THEN
            IF(LG(30)) THEN
                IF(INDVAR.NE.NPHI) RETURN
                L0FXG=L0F(XG2D)
                L0FYG=L0F(YG2D)
                L0VAL=L0F(VAL)
                DO 1100 IX=1,NX
                    DO 1100 IY=1,NY
                        I=IY + (IX-1)*NY
                        F(L0VAL+I)=RG(1)
                        XG=F(L0FXG+I)
                        YG=F(L0FYG+I)
                        IF((XG + 1.63177*YG).LT.XULAST*RG(6)) F(L0VAL+I)= RHO2
1100          CONTINUE
                    ENDIF
C  GROUP 13. Boundary conditions and special sources
C  =====
        ELSEIF(IGR.EQ.13) THEN
C  * ----- SECTION 12: GENTRA sources
        IF(ISC.EQ.12) THEN
            IF(NPATCH(1:6).EQ.'GENMAS'.OR.NPATCH(1:6).EQ.'GENPAT')
THEN
                IF(ISWEEP.GE.GSWEPI) THEN
                    IF(NPATCH(1:6).EQ.'GENMAS') THEN
C.....      Mass source
                        IF((INDVAR.EQ.P1).AND.STORE(MASS)) THEN
                            CALL FN0(VAL,MASS)
                            CALL GETCOV('GENMAS',1,GCOV,GVAL)
                            IF(QNE(GCOV,FIXFLU)) THEN
                                GMULT=1./GCOV
                                CALL FN25(VAL,GMULT)
                            ENDIF
                        ENDIF
                    ELSEIF(NPATCH(1:6).EQ.'GENPAT') THEN
C.....      Other interfacial sources
                        IF((INDVAR.EQ.U1).AND.STORE(MOMX)) THEN
                            CALL FN0(VAL,MOMX)
                        ELSEIF((INDVAR.EQ.V1).AND.STORE(MOMY)) THEN
                            CALL FN0(VAL,MOMY)
                        ELSEIF((INDVAR.EQ.W1).AND.STORE(MOMZ)) THEN
                            CALL FN0(VAL,MOMZ)

```

```

1          ELSEIF( ( INDVAR.EQ.H1.OR.INDVAR.EQ.JTEM1 ).AND.
              STORE(HEAT) ) THEN
              CALL FN0(VAL,HEAT)
              ELSEIF( ( INDVAR.EQ.VAPO ).AND.STORE(MASS) ) THEN
              CALL FN0(VAL,MASS)
              ENDIF
              ENDIF
              IF(.NOT.STEADY) CALL FN25(VAL,1.0/DT)
          ELSE
              CALL FN1(VAL,0.0)
          ENDIF
      ENDIF
  ENDIF
ENDIF
C
C
C GROUP 19. Special calls to GROUND from EARTH
C =====
C
      ELSEIF(IGR.EQ.19) THEN
C      * ----- SECTION 1 ---- START OF TIME STEP.
      IF(ISC.EQ.1) THEN
          LGSWEP=0
          PSTLSW=.FALSE.
          IF(ISTEP.EQ.1) THEN
C....      Domain size
              CALL SUB3R (XLASTM,XULAST,YLASTM,YVLAST,ZLASTM,ZWLAST)
              CELMIN=AMIN1(XLASTM/FLOAT(NX),YLASTM/FLOAT(NY),
$              ZLASTM/FLOAT(NZ))
C....      Find the axis
              CALL FNDAXI
          ENDIF
          CALL GENIUS (1,2)
C      * ----- SECTION 2 ---- START OF SWEEP.
      ELSEIF(ISC.EQ.2) THEN
C..      A. Index of first actual sweep.....
          IF(GFASWP.EQ.-9999) THEN
              GFASWP=ISWEEP
              GSWEPl=MAX0(GFASWP,GSWEPl)
          ENDIF
C..      B. Last sweep?.....
C      At least two sweeps are needed for one time step
          LSTSWP=( ISWEEP.GE.LSWEEP ).OR.(RESMET.AND.ISWEEP.GT.1)
          GENCAL=( ISWEEP.GE.GSWEPl ).AND.
+
          ((MOD(ISWEEP,GSWEPl).EQ.0).OR.(GSWEPl.EQ.ISWEEP).OR.LSTSWP)
C..      D. Reset sources .....
          IF(GENCAL) THEN
              DO 1921 IZZ=1,NZ
C....      Setting interphase sources to 0 in the first GENTRA
sweep
                  IF(ISWEEP.EQ.GSWEPl) THEN
                      IF(.NOT.LG(11).AND.NOTGXM.AND.IZZ.EQ.1) THEN
                          WRITE(BUFF(1),'(A)')
+                          'GENTRA resetting interphase sources to 0'
                          CALL PRINT_CHECK(BUFF,1,LUPRO)
                      ENDIF

```

```

        IF(STORE(MOMX)) THEN
            MOMXZ=ANYZ(MOMX,IZZ)
            CALL FN1(MOMXZ,0.0)
        ENDIF
        IF(STORE(MOMY)) THEN
            MOMYZ=ANYZ(MOMY,IZZ)
            CALL FN1(MOMYZ,0.0)
        ENDIF
        IF(STORE(MOMZ)) THEN
            MOMZZ=ANYZ(MOMZ,IZZ)
            CALL FN1(MOMZZ,0.0)
        ENDIF
        IF(STORE(HEAT)) THEN
            HEATZ=ANYZ(HEAT,IZZ)
            CALL FN1(HEATZ,0.0)
        ENDIF
        IF(STORE(MASS)) THEN
            MASSZ=ANYZ(MASS,IZZ)
            CALL FN1(MASSZ,1.0E-20)
        ENDIF
    ENDIF
    IF((GRESTI.NE.0).AND.LSTSWP).AND.STORE(REST)) THEN
        IF(LOOPZ.EQ.1) THEN
            JREST=ANYZ(REST,IZZ)
            CALL FN1(JREST,0.0)
        ENDIF
    ENDIF
1921    CONTINUE
        ENDIF
C      * ----- SECTION 3 ---- START OF IZ SLAB.
        ELSEIF(ISC.EQ.3) THEN
C      .....
C      PSICEL is the main particle-tracking module. It will
C      calculate the particle trajectories and the interphase
C      sources of momentum, heat and mass at each cell.
C      Its CALL is conditioned to GENCAL, set above
C      .....
C      PSICEL protected against double calling in the same sweep
        IF(.NOT.PSTLSW.AND.IZ.EQ.1.AND.GENCAL.AND.
+       ISWEEP.NE.LGSWEP) THEN
            IF(.NOT.LG(11).AND.NOTGXM) THEN
                WRITE(BUFF(1),'(A,I4)')
+       'GENTRA now tracking particles at sweep',ISWEEP
                CALL PRINT_CHECK(BUFF,1,LUPRO)
            ENDIF
            if(dbggen) then
                call writ8('GENTRA..')
                call writlr('TIME= ',TIM)
                call writli('ISWEEP',ISWEEP)
            endif
            CALL PSICEL
            IF(.NOT.LG(11).AND.NOTGXM) THEN
                IF(LUPRO.NE.6) THEN
                    WRITE(LUPRO,'(A)') 'GENTRA returns control to Earth'
                ELSE

```

```

CALL PUT_LINE('GENTRA returns control to
Earth',.true.)
ENDIF
ENDIF
IF(LSTSWP) PSTLSW=.TRUE.
LGSWEP=ISWEEP
ENDIF
C      * ----- SECTION 6 ---- FINISH OF IZ SLAB.
cc     ELSEIF(ISC.EQ.6) THEN
C      * ----- SECTION 7 ---- FINISH OF SWEEP.
ELSEIF(ISC.EQ.7) THEN
C...   Test whether the RESREF criterion was met before LSWEEP
CALL LASTSW
C      * ----- SECTION 8 ---- FINISH OF TIME STEP.
ELSEIF(ISC.EQ.8) THEN
IF(GHFILE(1:4).NE.'NONE') THEN
IF(.NOT.STEADY.AND.(NX.EQ.1.OR.NY.EQ.1.OR.NZ.EQ.1)) THEN
DO I= 1, NTRACK
ILOC0= IPFSTR(I)+IPRSTN
IWRT= ISTEP
IF(I.EQ.1) IWRT= -ISTEP
WRITE(LUHI, '(I4,A,11(1PE13.3))') IWRT, ' ',
+      TIM, (F(ILOC0+J),J=1, 10)
ENDDO
ENDIF
ENDIF
IF(LG(30)) THEN
LXU2D=L0F(XU2D)
LYV2D=L0F(YV2D)
L0C1=L0F(C1)
IFACE= IG(30)
CALL TRKDEN(F(L0C1+1),LXU2D,LYV2D,IFACE)
ENDIF
IF(GENCAL.AND.ISTEP.EQ.LSTEP) THEN
C....   write GENTRA restart file
IF(.NOT.STEADY.AND.NTRACK.GT.0) CALL WRSTRT
C....   GENTRA check
IF(LG(10)) THEN
RNTRAK=REAL(NTRACK)
RESIDL=0.0
ICK=6
IF(TSOLVE)ICK=7
IF(VAPSOL)ICK=8
DO 115 IS=1,ICK
IRG=50+IS
RESIDL=RESIDL+ABS((CHQ(IS)-RG(IRG))/(RG(IRG)+1.E-7))
115    CONTINUE
IF(RESIDL.GT.0.2) THEN
WRITE(BUFF(1), '(A)') 'CHECK !!'
WRITE(BUFF(2),1150)(50+IS,CHQ(IS),IS=1,6)
WRITE(BUFF(3),1160)(50+IS,CHQ(IS),IS=7,8)
CALL PRINT_CHECK(BUFF,3,LUPRO)
ENDIF
ENDIF
IF(LG(11)) THEN
IF(NOTGXM) CALL GRCLZZ

```

```

        CALL CLOSZZ(44)
        IF(LG(12)) CALL CLOSZZ(43)
    ENDIF
ENDIF
ENDIF
C=====
=====
    ENDIF
1150 FORMAT(2('RG(',I2,')=',1PE9.2,',';'),'RG(',I2,')=',1PE9.2)
1160 FORMAT('RG(',I2,')=',1PE9.2,',';RG(',I2,')=',1PE9.2)
    END
C
C
.....1.....2.....3.....4.....5.....6.....
7.....8
C
C-----
-----
c
C Subroutine GENIUS:
C GENTra Interface for User Sequences
C ===      =          =          =
C
C Examples included:
C GENEX1: Time-step statistics
C GENEX2: Automatic generation of USE file for PHOTON
C-----
-----
    SUBROUTINE GENIUS (IGENGR, IGENSC)
C....Earth and GENTRA data imported via COMMONs in INCLUDE
C    files
C    INCLUDE '/phoenics/d_includ/satear'
C    INCLUDE '/phoenics/d_includ/grdloc'
C    INCLUDE '/phoenics/d_includ/satgrd'
C    INCLUDE '/phoenics/d_includ/grdear'
C    INCLUDE '/phoenics/d_includ/grdbfc'
C    INCLUDE '/phoenics/d_includ/bfcear'
C    INCLUDE '/phoenics/d_includ/tracmn'

C=====
=====
C
C
C GROUP 1: Preliminaries
C    =====
C    IF(IGENGR.EQ.1) THEN
C        * ----- Section 1: Beginning of current PHOENICS
session
C        The property index used to identify solid region (INTEGER)
C        in conjugate-heat transfer cases. Consult CHAM if uncertain.
        PRINDX=100
        IF(IGENSC.EQ.1) THEN
C            * ----- Section 2: Beginning of current Eulerian
time step
                ELSEIF(IGENSC.EQ.2) THEN
                    ENDIF

```

```

C
C GROUP 2: Start of new track
C      =====
C      ELSEIF(IGENGR.EQ.2) THEN
C
C GROUP 3: Start of new Lagrangian time-step for the current track
C      =====
C
C      ELSEIF(IGENGR.EQ.3) THEN
C        IF(LG(30)) THEN
C          IF(IP.EQ.1) THEN
C            UCPARN= 0.0
C            VCPARN= 0.73*UCGASN
C          ELSEIF(IP.EQ.NTRACK) THEN
C            UCPARN= UCGASN
C            VCPARN= 0
C          ENDIF
C        ENDIF
C
C GROUP 4: Particle reaches cell boundary
C      =====
C      ELSEIF(IGENGR.EQ.4) THEN
C        -----
C      ----
C      IGENSC values as follows:
C      1-Exit      2-Wall      3-Axis or symmetry surface      4-New cell
C      -----
C      ----
C
C GROUP 5: End of the current Lagrangian time step
C      =====
C      ELSEIF(IGENGR.EQ.5) THEN
C
C GROUP 6: End of current track
C      =====
C      ELSEIF(IGENGR.EQ.6) THEN
C
C GROUP 7: GENTRA returns control to Earth
C      =====
C      ELSEIF(IGENGR.EQ.7) THEN
C
C GROUP 8: Special calls
C      =====
C      ELSEIF(IGENGR.EQ.8) THEN
C        IF(IGENSC.EQ.1) THEN
C          * ----- Section 1: Momentum equation
C          Give constants GVCSCX, GVCSCY and GVCSCZ
C          in the energy equation
C
C
C          / Up /          / Ug /          / Up /      / GVCSCX
C          /
C          d |      |      |      |      |      |      |
C          |
C          ----| Vp | = GVCSCB*| Vg | - GVCSCA*| Vp | + | GVCSCY
C          |

```



```

C          dt |      |      |      |      |      |
C          / Wp /      / Wg /      / Wp /      / GVCSCZ
C
C
C          Up
C          Vp : The particle velocity
C          Wp
C
C          Ug
C          Vg : The gas velocity
C          Wg
C
C      ELSEIF(IGENSC.EQ.2) THEN
C          * ----- Section 2: Energy equation
C          Give constants GHCSAA, GHCSBB and GHSCC
C          in the energy equation
C
C              dTp
C          ----- = GHCSBB*Tgas - GHCSAA*Tp + GHSCC
C              dt
C
C          M: Particle mass
C          T: Temperature
C
C          The default setting:
C              A=B1=interface heat transfer coefficient
C              B1=Latent heat du to evaporation
C          Disregarding default setting by reseting A, B1 and B2 to
C          zero.
C
C      ELSEIF(IGENSC.EQ.3) THEN
C          * ----- Section 3: Particle mass equation
C
C              dD**2
C          ----- = [GMCSAA]-[GMCSAA]*(D**2)
C              dt
C
C          D: Particle diameter
C
C
C      ELSEIF(IGENSC.EQ.4) THEN
C          * ----- Section 4: Formulation for solidification
C
C              d(Mass frac. of solid)
C          ----- = [GHCSAA]
C              d(Temper. of part.)
C
C
C      ELSEIF(IGENSC.EQ.5) THEN
C          * ----- Section 5: User's equations
C      ENDIF
C
C      GROUP 9: Particle inlet condition as function of time (TIM)
C          =====

```

```

        ELSEIF(IGENGR.EQ.9) THEN
C...      PRVLIN=?
C
C...      * ----- Section 1: Particle X-coordinate
        IF(IGENSC.EQ.1) THEN
            PRVLIN=2.*TIM
C
C...      * ----- Section 2: Particle Y-coordinate
        ELSEIF(IGENSC.EQ.2) THEN
            PRVLIN=1.0
C
C...      * ----- Section 3: Particle Z-coordinate
        ELSEIF(IGENSC.EQ.3) THEN
            PRVLIN=0.2
C
C...      * ----- Section 4: Particle U-velocity (Cartesian
components)
        ELSEIF(IGENSC.EQ.4) THEN
            PRVLIN=0.1
C
C...      * ----- Section 5: Particle V-velocity (Cartesian
component)
        ELSEIF(IGENSC.EQ.5) THEN
            PRVLIN=0.1
C
C...      * ----- Section 6: Particle W-velocity (Cartesian
component)
        ELSEIF(IGENSC.EQ.6) THEN
            PRVLIN=2.0
C
C...      * ----- Section 7: Particle diameter
        ELSEIF(IGENSC.EQ.7) THEN
            PRVLIN=0.001
C
C...      * ----- Section 8: Liquid density of particle
        ELSEIF(IGENSC.EQ.8) THEN
            PRVLIN=1000.0
C
C...      * ----- Section 9: Mass flow pass particle inlet
(Nozzle etc.)
        ELSEIF(IGENSC.EQ.9) THEN
            PRVLIN=0.1
C
C...      * ----- Section 10: Number of identical particle
parcels.
        ELSEIF(IGENSC.EQ.10) THEN
C
C...      * ----- Section 11: Particle temperature
        ELSEIF(IGENSC.EQ.12) THEN
            PRVLIN=350.0
C
C...      * ----- Section 12: Density of the solid
        ELSEIF(IGENSC.EQ.13) THEN
            ENDIF
C

```

```

C=====
=====
C      ENDIF
C      END
C
C
C      FUNCTION GPROPS(FUNAME, PARAMT, DEFVAL)
C-----
C      Functions to calculate liquid and gas properties for GENTRA
C      Only one parameter is permitted for each function. others
C      are passed through 'TRACMN'
C
C      FUNAME:      character string      name of the function
C      PARAMT:      real                  parameter of the function
C      DEFVAL:      real                  default value
C-----
C
C      INCLUDE '/phoenics/d_includ/satear'
C      INCLUDE '/phoenics/d_includ/tracmn'
C      INCLUDE '/phoenics/d_includ/grdloc'
C      INCLUDE '/phoenics/d_includ/satgrd'
C      INTEGER FUNAME
C      LOGICAL FINDGR,GRN
C      CHARACTER*80 BUFF
C      if(dbglev.and.dbgrnd) then
C          call writli('findx:',funame)
C          call writ2r('paramt',paramt,'defval',defval)
C      endif
C
C-----
C      Default value or Q1-set flag
C-----
C      GPROPS=DEFVAL
C
C=====      GROUND 1: WATER AND AIR      =====
C
C      IF(GRNDNO(1,DEFVAL)) THEN
C
C          IF(FUNAME.EQ.1) THEN
C-----
C          1  Drag coefficient
C-----
C
C          gprops = drag coefficient
C          defval = q1-set flag
C          paramt = particle Reynolds number
C.....      Law for spherical particles
C          GPROPS=(24.0/PARAMT)*(1.0 + 0.15*PARAMT**0.687)+
C          +      (0.42/(1. + (4.25E + 4*PARAMT**(-1.16))))
C          ELSEIF(FUNAME.EQ.2) THEN
C-----
C          2  Nusselt number
C-----
C
C          gprops = Nusselt number
C          defval = q1-set flag
C          paramt = particle Reynolds number
C

```

```

C.... Prandtl number
      IF(STORE(H1)) THEN
        PRNDT=PRNDTL(H1)
      ELSEIF(STORE(JTEM1)) THEN
        PRNDT=PRNDTL(JTEM1)
      ENDIF
      IF(GRN(-ABS(PRNDT)) .OR. PRNDT.LT.0.0) PRNDT= 0.7
      GPROPS=2.0+0.6*SQRT(PARAMT)*PRNDT**0.3333
C.... Froessling Number
      GPRFFF=1.0
      IF(VAPSOL.AND.GPRYVS.LT.1.0) THEN
        GBM=(GPRYVS-GCONGS)/(1.0-GPRYVS)
        IF(GBM.GT.1.E-05)GPRFFF=ALOG(1.0+GBM)/GBM
      ENDIF
      GPROPS=GPRFFF*GPROPS
      ELSEIF(FUNAME.EQ.3) THEN
C-----
C      3 Thermal conductivity of cont. phase.(without vapour)
C-----
C      gprops = thermal conductivity of pure continuous phase
C      paramt = temperature of the continuous phase
      ELSEIF(FUNAME.EQ.4) THEN
C-----
C      4 Thermal conductivity of vapour
C-----
C      gprops = thermal conductivity of vapour
C      paramt = particle temperature
C
      GPROPS=10.0**(9.1E-04*(PARAMT - 373.0) + 1.39)/1000.0
      ELSEIF(FUNAME.EQ.5) THEN
C-----
C      5 Latent heat of solidification
C-----
C      gprops = latent heat of solidification
C      paramt = particle temperature
C
      ELSEIF(FUNAME.EQ.6) THEN
C-----
C      6 Temperature of cont. phase as a function of enthalpy
C-----
C      gprops = temperature of the continuous phase
C      paramt = enthalpy of the continuous phase
      GPROPS=PARAMT/GCPGAS
      ELSEIF(FUNAME.EQ.7) THEN
C-----
C      7 Enthalpy of cont. phase as a function of temperature
C-----
C      gprops = enthalpy of the continuous phase
C      paramt = temperature of the continuous phase
      GPROPS=(PARAMT-TMP1A)/TMP1B
      ELSEIF(FUNAME.EQ.8) THEN
C-----
C      8 Heat capacity (Cp) of the particle
C      (Cp of liquid for melt/solidif. particle)
C-----
C      gprops = heat capacity of the particle

```

```

C          (Cp of liquid for melt/solidif. particle)
C      paramt = particle temperature (Kelvin)
C      XPARAM=PARAMT/273.15
C      GPROPS=-3892.438*XPARAM**3 + 14895.93*XPARAM**2
C      +
C          -18779.6*XPARAM + 11993.33
C      ELSEIF(FUNAME.EQ.9) THEN
C-----
C      9 Latent heat of evaporation
C-----
C      gprops = latent heat of evaporation
C      paramt = temperature of the particle
C      Derived from curve fit on steam tables (T in Kelvin)
C      GPROPS=6.2909E+06 - 2.7457E+4*PARAMT + 65.991*PARAMT**2
C      +
C          - 5.7653E - 2*PARAMT**3
C      ELSEIF(FUNAME.EQ.10) THEN
C-----
C      10 Solid fraction
C-----
C      gprops = solid fraction
C      paramt = temperature of the particle
C      GPROPS=0.0
C      GBASE= (GTLIQD-PARAMT)/(GTLIQD-GTSOLD)
C      IF(GBASE.GT.0.0)GPROPS=GBASE**GMINDX
C      IF(PARAMT.LE.GTSOLD) GPROPS=1.0
C      ELSEIF(FUNAME.EQ.11) THEN
C-----
C      11 Index of solid-fraction formula
C-----
C      gprops = index of solidification formula
C      paramt = local pressure of the continuous phase
C
C      ELSEIF(FUNAME.EQ.12) THEN
C-----
C      12 Density of the particle
C-----
C      gprops = density of particle (for liquid only if GTYPE=50)
C      paramt = temperature of the particle
C      GPROPS=1000.0
C      ELSEIF(FUNAME.EQ.13) THEN
C-----
C      13 Density of the solid phase of the particle
C-----
C      gprops = density of solid
C      paramt = temperature of the solid
C
C      ELSEIF(FUNAME.EQ.14) THEN
C-----
C      14 Saturation press. of vapour.
C-----
C      gprops = saturation pressure
C      paramt = temperature of the liquid
C
C      (Vapour-pressure correlation of Bain [1964]
C      Convert from degree Kelvin to Degrees Celcius)
C      TCLCIS=AMAX1(PARAMT-273.15,1.0)
C      Convert Tsat from degC to degR

```

```

TDEGR=1.8*TCLCIS+492.
IF(TDEGR.LE.672.0) THEN
C      Correlation for T <= 100 degC
      TDEGR1=73.32642 - 8.2*ALOG(TDEGR)
      +      + 0.003173*TDEGR - 13023.8/TDEGR
ELSE
C      Correlation for 100 degC <= Tcrit
      ZZZ=TDEGR*TDEGR-951588.
C.... No super-critical state is included
      HHH=AMAX1(1165.09 - TDEGR,0.0)
      CONS2=2.624453E-12*ZZZ*ZZZ
      IF(CONS2.GT.50.) CONS2=50.
      CONS3=-0.00631141*HHH**1.25
      IF(CONS3.LT.-50.) THEN
        CONS3=-50.
      ELSEIF(CONS3.GT.50.) THEN
        CONS3=50.
      ENDIF
      TDEGR2=0.00017741*ZZZ*(EXP(CONS2)-1.)/TDEGR
      TDEGR3=-0.01013139*EXP(CONS3)
      TDEGR1=15.182911-8310.453/TDEGR+TDEGR2+TDEGR3
ENDIF
C      Convert Psat from lbf/in2 to N/m2 by multiplying by
6894.76
      IF(TDEGR1.GT.50.) TDEGR1=50.
      IF(TDEGR1.LT.-50.) TDEGR1=-50.
      GPROPS=EXP(TDEGR1)*6894.76
      ELSEIF(FUNAME.EQ.15) THEN
C-----
C      15 Heat capacity (Cp) of vapour
C-----
C      gprops = heat capacity of vapour
C      paramt = temperature
C      Cp is calculated under saturation condition
C      The temperature should be higher than 100 degree C.
      TEMQ=AMAX1(PARAMT-273.15,100.0)
      GPROPS=1.2745E-07*TEMQ**5-1.2475E-04*TEMQ**4
      +      +4.7457E-02*TEMQ**3-8.7110*TEMQ**2+773.98*TEMQ-2.4505E+04
      ELSEIF(FUNAME.EQ.16) THEN
C-----
C      16 Cp of the continuous phase (without vapour).
C-----
C      gprops = heat capacity of pure continuous phase
C      paramt = temperature of the gas
C
      ELSEIF(FUNAME.EQ.17) THEN
C-----
C      17 Solidus temperature
C-----
C      gprops = saturation temperature of solidification
C      paramt = pressure of cont. phase
C
      ELSEIF(FUNAME.EQ.18) THEN
C-----
C      18 Liquidus temperature
C-----

```

```

C      gprops = saturation temperature of cont. phase
C      paramt = pressure of cont. phase
C
      ELSEIF(FUNAME.EQ.19) THEN
C-----
C      19 Particle enthalpy
C      (liquid enthalpy for melt/solidif. particle)
C-----
C      gprops = particle enthalpy
C      (liquid enthalpy for melt/solid. part.)
C      paramt = particle temperature
C
      XPARAM=PARAMT/273.15
      GPROPS=-1.80172E+06-
265805.0*XPARAM**4+1.35627E+06*XPARAM**3
      +      -2.56482E+06*XPARAM**2+3.27598E+06*XPARAM
C
      ELSEIF(FUNAME.EQ.20) THEN
C-----
C      20 Vapour saturation temperature as function of pressure
C-----
C      gprops = saturation temperature
C      paramt = pressure of the continuous phase
C
      XPARAM=ALOG(PARAMT)-5.0

GPROPS=0.31911*XPARAM**3+3.1032*XPARAM**2+27.287*XPARAM+370.8
C
      ELSEIF(FUNAME.EQ.21) THEN
C-----
C      21 Cp of solid for solidifying/melting particle
C-----
C      gprops = heat capacity of solid
C      paramt = particle temperature
C
      ENDIF
C=====
C=====
C
C
C=====
C=====
C
C      Example functions used for testing and validation.
C
      ELSEIF(GRNDNO(2,DEFVAL)) THEN
      IF(FUNAME.EQ.5) THEN
C-----
C      5 Latent heat of solidification
C-----
C      gprops = latent heat of solidification
C      paramt = particle temperature
C
      GPROPS=-1.3E+06 + 1000.0*PARAMT
      ELSEIF(FUNAME.EQ.8) THEN

```

```

C-----
C      8  Heat capacity (Cp) of the particle
C-----
C      gprops = heat capacity of the liquid
C      paramt = liquid temperature (Kelvin)
C      GPROPS=1000.0 + 0.1*PARAMT
C      ENDIF

C
C=====                                GROUND   X:   (           )
=====
C      ELSEIF(GRNDNO(X,DEFVAL)) THEN
C-----
C      Properties for other materials can be added in exactly the
C      same way as for water. X is from 1 to 10 and GRNDX should
be
C      given to the request property as default in Q1.
C-----
C      ENDIF
C      ENDIF

C=====                                END      =====
C
C      IF(FINDGR(GPROPS)) THEN
C      WRITE(BUFF,'(A,I2,A)')'GPROPS ',FUNAME,
+ ' ' is required but no constant or function has been supplied
!'
C      CALL PRINT_CHECK(BUFF,1,LUPRO)
C      CALL GWYOUT(2)
C      ENDIF
C      if(dbglev.and.dbgrnd) call writlr('gprops',gprops)
C      END
c

```


Appendix H. The GENTRA Glossary

The GENTRA Glossary contains a summary of the main terms used in Gentra and its documentation. It is also available interactively through the GENTRA Input Menu (See Section 2.5).

GENIUS

GENIUS (GENtra Interface for User Sequences) is a user-accessible FORTRAN-module where GENTRA users can insert their own coding sequences to replace and supplement the built-in physical laws, numerical devices and output options.

GENTRA

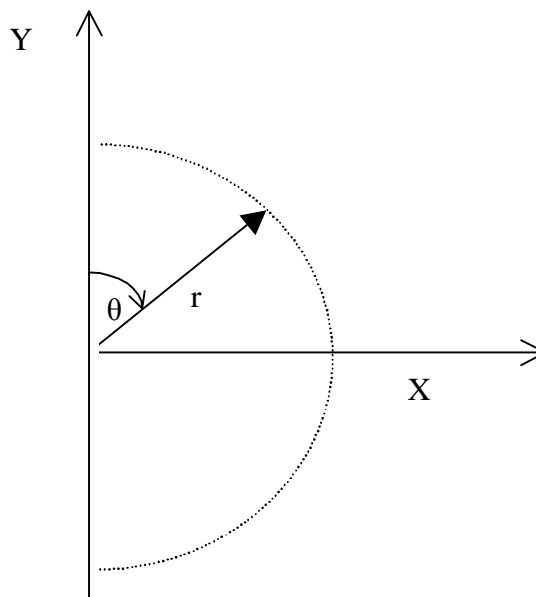
Particle-tracking software for the PHOENICS flow-simulation package. GENTRA consists of:-

- The GENTRA Menu, a collection of data files to be used with the PHOENICS-SATELLITE pre-processor;
- The GENTRA GROUND, a PHOENICS-EARTH GROUND-Station which contains the tracking routines.

GENTRA CARTESIAN SYSTEM

GENTRA uses, for the integration of the particle equations, a Cartesian co-ordinate system. This system is related to the PHOENICS grid system as follows:-

- For Cartesian grids, both systems are identical.
- For BFC grids, the GENTRA Cartesian system is the same Cartesian system used in PHOENICS to define the grid corners.
- For cylindrical-polar grids, the relationship between both systems is depicted in the figure:



The Z axes of the two systems coincide, forming a right-handed grid in each case.

The relationships connecting the two co-ordinate systems are:

$$X_c = R + r \cos (X_p)$$

$$Y_c = R + r \sin (X_p)$$

$$U_c = V_p \cos (X_p) - U_p \sin (X_p)$$

$$V_c = U_p \cos (X_p) + V_p \sin (X_p)$$

where $R = YV_{LAST}$.

OBSTACLES

(See WALLS)

PARCEL

The term PARCEL is used to refer to a group of particles that are injected at the same time, at the same position and with the same properties. The parcel is characterised by a MASS FLOW-RATE (kg/s), which specifies (together with the particle size, density and velocity) the number of particles in the parcel.

WALLS (AND OBSTACLES)

Walls and obstacles are defined in GENTRA (as in the rest of PHOENICS) through face and cell porosities (see the CONPOR command in the PHOENICS Reference Manual). The level of porosity that will be considered by GENTRA to be an obstruction for the particles can be set by the user; see the option POROSITY THRESHOLD in the BOUNDARY CONDITIONS panel.

Appendix I. References

I.1 Quoted in this guide

- R Clift, J R Grace, M E Weber (1988)
'Bubbles, Drops and Particles'
Academic Press, New York.
- C T Crowe, M P Sharma and D E Stock (1977)
'The Particle-Source-In-Cell Model for Gas-Droplet Flows'
ASME J. Fluids Eng., pp 325-332
- G M Faeth (1983)
'Evaporation and Combustion of Sprays'
Prog. Energy Comb. Sci., Vol. 9, pp 1-76
- A D Gosman and E Ioannides (1981)
'Aspects of Computer Simulation of Liquid-fuelled Combustors'
AIAA-81-0323, AIAA 19th Aerospace Sciences Meeting, St. Louis, Missouri, USA.
- D B Spalding (1980)
'Numerical Computation of Multiphase Fluid Flow and Heat Transfer'
Recent Advances in Numerical Methods in Fluids,
Ed. C Taylor and K Morgan, pp 139-167

I.2 Relevant CHAM Technical Reports

- CHAM TR324, Starting with PHOENICS-VR
- CHAM TR326, PHOENICS-VR Reference Guide
- CHAM TR99, The PHOENICS Equations

Appendix J. Nomenclature

Note: *Bold typeface indicates vector*

A_p Particle projected area [E6.7]

b Buoyancy factor [E6.5]

B_m Mass transfer number

C_D Drag coefficient [E6.8]

C_p Specific heat capacity

D_p Drag function [E6.6]

F Frössling correction for mass transfer

F_s Particle solid fraction

g Gravitational acceleration (vector)

H_{fg} Latent heat of vaporisation

K Turbulence kinetic energy

k Thermal conductivity

L Latent heat of solidification

m_p Mass of a particle

Nu Nusselt number

Re Particle Reynolds number ($Re = \frac{|\mathbf{U}_p - \mathbf{U}_c|d_p}{\nu_c}$)

T Temperature

T_L Liquidus temperature

T_s Solidus temperature

W Molecular weight

m Solidification index

Δt_e Eddy lifetime [E6.10]

Δt_r Eddy crossing-time [E6.12]

Δt_e Lagrangian time-step

α Particle heat transfer coefficient

U Instantaneous continuous-phase velocity

\mathbf{U}'_c Fluctuating continuous-phase velocity (Section 6.6.1)

\mathbf{U}_c Continuous-phase velocity

\mathbf{U}_p Particle velocity

\mathbf{x}_p Particle position

Y_{vs} Mass fraction of vapour at droplet surface

$Y_{v\infty}$ Mass fraction of vapour in surroundings

ε Rate of dissipation of turbulence kinetic energy

ϕ_c Continuous-phase property

Ω Angular speed of rotation of the co-ordinate system [E6.13]

ν_c Continuous-phase kinematic viscosity

ρ Density

Subscripts

p particle

v vapour

s particle solid phase

l particle liquid phase

c continuous phase

Appendix K. GENTRA Utilities

K.1 Plotting Trajectories

K1.1 In the Viewer

The particle trajectories can be plotted in the Viewer by using the global history file ("ghis" by default) as a macro. Click on **Macro** on the hand-set or **M** on the tool bar. On the dialog that opens, enter the name of the global history file as the Macro file and click 'OK' to run it. All the tracks in the file will be read and displayed as Viewer streamlines. They can then be turned on and off through the Streamline Management Dialog.

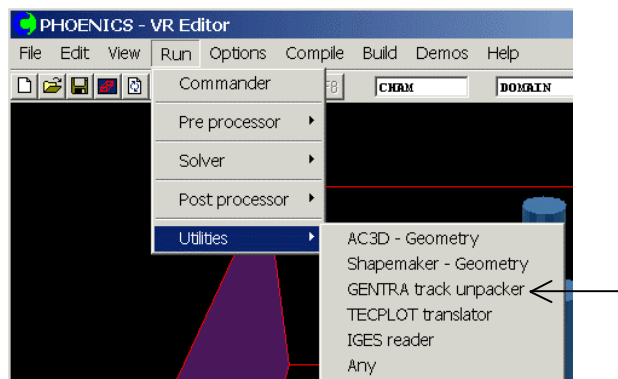
To plot individual tracks from the history file, create a macro file which contains the lines:

```
HISTORY READ
Filename m [,n]
```

where filename is the name of the history file, and n is the number of the track to draw. If m is present, all tracks in the range m-n will be drawn.

K.1.2 Running UNPACK

The track unpacking program, UNPACK, is run by clicking on **Run, Utilities, GENTRA track unpacker**. This is required to create individual history files for plotting in AUTOPLOT, but is NOT needed for the Viewer.



- * Start the track unpacker as described above.

The track unpacker assumes that the name of the global history file has not been changed from the default name ("ghis"). The single-character identifiers for the names of the individual history and trajectory files must now be specified. Typing "none" will deactivate the production of one or other (or both) of the file types.

- * In this example, we may want only history files (for viewing in AUTOPLOT) so type "none h" to prevent creation of trajectory files and to indicate that the name of the history files are to commence with "h".

The particular tracks for which files are to be produced must now be specified. These files can be specified by the individual track number (e.g. 3-4). Combinations of numbers and range up to a maximum of 20 inputs can be accepted (e.g. 1 3 5-7 10-12 14).

- * Continuing with the worked example for which five tracks are produced, if we want to produce history files for tracks 1, 3 and 4 we can input 1 3 4 or 1 3-4.

The resulting history files, called h00001, h00003 or h00004 can now be plotted in AUTOLOT.

If trajectory files are produced, a GENUSE file which plots them will also be written.

K.2 Saving as a case

The global history file, ghis, will be automatically saved as 'case.his', by clicking on **File, Save as a case**. The genuse file will be saved as 'case.gen'. The individual trajectory and history files will not be saved automatically. They can always be recovered from ghis by running the track unpacker, as described above.